DOE/ER-0509P

# ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 1990

May 31, 1991

**Annual Technical Report**

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

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Washington, D.C. 20585

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# INTRODUCTION

The DOE Energy Materials Coordinating Committee (EMaCC) serves primarily to enhance coordination among the Department's materials programs and to further the effective use of materials expertise within the Department. These functions are accomplished through the exchange of budgetary and planning information among program managers and through technical meetings/workshops on selected topics involving both DOE and major contractors. Four topical subcommittees are established and are continuing their own programs: Structural Ceramics, Electrochemical Technologies, Radioactive Waste Containment, and Superconductivity. In addition, the EMaCC aids in obtaining materials-related inputs for both intra- and inter-agency compilations.

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

The EMaCC reports to the Director of the Office of Energy Research in his capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC terms of reference. This report summarizes EMaCC activities for FY 1990 and describes the materials research programs of various offices and divisions within the Department.

The Chairman of EMaCC for FY 1990 was Scott L. Richlen; the Executive Secretary was Dr. Jerry Smith.

Dr. Jerry Smith
Office of Basic Energy Sciences
Chairman of EMaCC, FY 1991

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

| Organization | Representative | Phone No. |
|---|---|---|
| **CONSERVATION AND RENEWABLE ENERGY** | | |
| Building Technologies | | |
| Building Systems and Materials | Peter Scofield, CE-421 | 202/586-9193 |
| Building Equipment | John Ryan, CE-422 | 202/586-9130 |
| | Ronald Fiskum, CE-422 | 202/586-9130 |
| Industrial Technologies | | |
| Industrial Energy Efficiency | Scott Richlen, CE-221 | 202/586-2078 |
| Waste Materials Management | Donald Walter, CE-222 | 202/586-8072 |
| | Frank Wilkins, CE-222 | 202/586-1684 |
| Improved Energy Productivity | Matthew McMonigle, CE-231 | 202/586-2082 |
| | David Pellish, CE-231 | 202/586-6436 |
| Advanced Industrial Materials | Marvin E. Gunn, CE-232 | 202/586-5377 |
| Transportation Technologies | | |
| Advanced Transportation Materials | James Eberhardt, CE-34 | 202/586-5377 |
| | Robert B. Schulz, CE-34 | 202/586-8051 |
| Utility Technologies | | |
| Wind/Hydro/Ocean Technologies | William Richards, CE-121 | 202/586-5410 |
| Geothermal Technology | Raymond LaSala, CE-122 | 202/586-4198 |
| Photovoltaic Technology | Morton B. Prince, CE-131 | 202/586-1725 |
| Advanced Utility Concepts | Russell Eaton, III, CE-142 | 202/586-2826 |
| | Eberhart Reimers, CE-142 | 202/586-4563 |

## MEMBERSHIP LIST (Continued)

| Organization | Representative | Phone No. |
|---|---|---|
| **ENERGY RESEARCH** | | |
| Basic Energy Sciences | | |
| Materials Sciences | Iran L. Thomas, ER-13 | 301/353-3426 |
| Metallurgy and Ceramics | Robert J. Gottschall, ER-131 | 301/353-3428 |
| Solid State Physics and Materials Chemistry | B. Chalmers Frazer, ER-132 | 301/353-3426 |
| | Jerry Smith, ER-132 | 301/353-3426 |
| Engineering and Geosciences | Oscar P. Manley, ER-15 | 301/353-5822 |
| Advanced Energy Projects | Walter Polansky, ER-16 | 301/353-5995 |
| Health and Environmental Research | | |
| Physical and Technological Research | Gerald Goldstein, ER-74 | 301/353-5348 |
| Fusion Energy | | |
| Fusion Technologies | F. W. (Bill) Wiffen, ER-533 | 301/353-4963 |
| **NUCLEAR ENERGY** | | |
| Uranium Enrichment | | |
| Advanced Technology Projects/ Technology Transfer | Arnold Litman, NE-35 | 301/353-5777 |
| Civilian Reactor Development | | |
| Advanced Reactor Programs | Andrew Van Echo, NE-45 | 301/353-3930 |
| | J. Edward Fox, NE-451 | 301/353-3985 |

## MEMBERSHIP LIST (Continued)

| Organization | Representative | Phone No. |
| --- | --- | --- |
| Space and Defense Power Systems | | |
| Special Applications | William Barnett, NE-53 | 301/353-3097 |
| | Arthur S. Mehner, NE-53 | 301/353-4474 |
| Naval Reactors | Robert H. Steele, NE-60 | 703/603-5565 |
| Nuclear Safety Self-Assessment | | |
| Nuclear Quality Assurance | Benjamin C. Wei, NE-84 | 301/353-3927 |
| **ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT** | | |
| Waste Operations | | |
| Waste Management Projects | Mark Frei, EM-34 | 301/353-7201 |
| | Henry F. Walter, EM-34 | 301/353-7192 |
| | Ken Chacey, EM-34 | 301/353-7186 |
| Technology Development | | |
| Research and Development | Kathleen Hain, EM-54 | 301/353-7917 |
| | Stanley M. Wolf, EM-54 | 301/353-7962 |
| **DEFENSE PROGRAMS** | | |
| Research and Advanced Technology | | |
| Research and Technology Development | Carl B. Hilland, DP-242 | 301/353-3687 |
| Inertial Confinement Fusion | Robert A. Jones, DP-243 | 301/353-5492 |

## MEMBERSHIP LIST (Continued)

| Organization | Representative | Phone No. |
|---|---|---|
| FOSSIL ENERGY | | |
| Management, Fundamental Research, and Cooperative Development | | |
| Technical Coordination | James P. Carr, FE-14 | 301/353-6519 |

## ORGANIZATION OF THE REPORT

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

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

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

The FY 1990 Budget Summary Table for materials activities in each of the programs within the DOE is presented on pages 7-9.

## FY 1990 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 1990 |
|---|---|
| **Office of Building Technologies** | $ 860,000 |
| Office of Building Energy Research | 860,000 |
| Buildings Systems and Materials Division | 860,000 |
| **Office of Industrial Technologies** | $17,668,000 |
| Office of Waste Reduction Technologies | 6,251,000 |
| Industrial Energy Efficiency Division | 2,788,000 |
| Waste Material Management Division | 3,463,000 |
| Office of Industrial Processes | 11,417,000 |
| Improved Energy Productivity Division | 1,732,000 |
| Advanced Industrial Concepts Division | 9,685,000 |
| **Office of Transportation Technologies** | $26,801,000 |
| Office of Transportation Materials | 15,036,000 |
| Office of Propulsion Systems | 11,765,000 |
| Office of Alternative Fuels | 0 |
| **Office of Utility Technologies** | $33,847,788 |
| Office of Solar Energy Conversion | 19,250,000 |
| Solar Thermal and Biomass Power Division | 850,000 |
| Photovoltaic Energy Technology Division | 18,400,000 |

## FY 1990 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

| | FY 1990 |
|---|---|
| **Office of Utility Technologies (Continued)** | |
| Office of Renewable Energy Conversion | 599,700 |
| Geothermal Technology Division | 599,700 |
| Office of Energy Management | 13,998,088 |
| Utility Systems Division | 125,000 |
| Advanced Utility Concepts Division | 13,873,088 |
| **Office of Energy Research** | $227,437,657 |
| Office of Basic Energy Sciences | 205,653,806 |
| Division of Materials Sciences | 198,400,000 |
| Division of Engineering and Geosciences | 6,481,806 |
| Division of Advanced Energy Projects | 772,000 |
| Office of Fusion Energy | 0* |
| Small Business Innovation Research Program | 21,783,851 |
| **Office of Environmental Restoration and Waste Management** | $ 10,750,000 |
| Division of Waste Management Projects | 10,750,000 |

*No submission was received from this office for FY 1990.

## FY 1990 BUDGET SUMMARY TABLE FOR DOE MATERIALS ACTIVITIES (Continued)

| | FY 1990 |
|---|---|
| **Office of Nuclear Energy** | $128,634,000 |
| Office of Uranium Enrichment | 20,513,000 |
| Office of Civilian Reactor Development | 29,786,000 |
| Office of Advanced Reactor Programs | 3,430,000 |
| Division of High Temperature Gas-Cooled Reactors | 3,430,000 |
| Office of Technology Support Programs (LMRs) | 26,356,000 |
| Office of Space and Defense Power Systems | 1,335,000 |
| Office of Naval Reactors | 77,000,000* |
| **Office of Civilian Radioactive Waste Management** | $ 12,640,100 |
| Office of Civilian Radioactive Waste Management/Yucca Mountain Site-Characterization Project Office (OCRWM/YMPO) | 12,640,100 |
| **Office of Defense Programs** | $ 42,761,000 |
| Office of Research and Advanced Technology | 42,761,000 |
| Research and Technology Division | 42,761,000 |
| **Office of Fossil Energy** | $ 7,031,000 |
| Office of Technical Coordination | 7,031,000 |
| Office of Coal Technology | 0 |
| Division of Clean Coal Technology | 0 |
| **TOTAL** | **$508,430,545** |

*Approximate

## 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 1990 budgets for each. More details on the individual projects within the divisions and the specific tasks or subcontracts within the various projects are given in the paragraph descriptions.

## OFFICE OF CONSERVATION AND RENEWABLE ENERGY

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

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

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

| | FY 1990 |
|---|---|
| 1. Office of Building Technologies | $ 860,000 |
| a. Office of Building Energy Research | 860,000 |
| (1) Buildings Systems and Materials Division | 860,000 |
| 2. Office of Industrial Technologies | $17,668,000 |
| a. Office of Waste Reduction Technologies | 6,251,000 |
| (1) Industrial Energy Efficiency Division | 2,788,000 |
| (2) Waste Material Management Division | 3,463,000 |
| b. Office of Industrial Processes | 11,417,000 |
| (1) Improved Energy Productivity Division | 1,732,000 |
| (2) Advanced Industrial Concepts Division | 9,685,000 |
| 3. Office of Transportation Technologies | $26,801,000 |
| a. Office of Transportation Materials | 15,036,000 |
| b. Office of Propulsion Systems | 11,765,000 |

| | | FY 1990 |
|---|---|---|
| 4. | Office of Utility Technologies | $33,847,788 |
| a. | Office of Solar Energy Conversion | 19,250,000 |
| | (1) Solar Thermal and Biomass Power Division | 850,000 |
| | (2) Photovoltaic Energy Technology Division | 18,400,000 |
| b. | Office of Renewable Energy Conversion | $ 599,700 |
| | (1) Geothermal Technology Division | 599,700 |
| c. | Office of Energy Management | 13,998,088 |
| | (1) Utility Systems Division | 125,000 |
| | (2) Advanced Utility Concepts Division | 13,873,088 |

## OFFICE OF BUILDING TECHNOLOGIES

| | FY 1990 |
|---|---|
| Office of Building Technologies - Grand Total | $860,000 |
| Office of Building Energy Research | $860,000 |
| Building Systems and Materials Division | $860,000 |
| Materials Properties, Behavior, Characterization or Testing | $860,000 |
| Unguarded Thin Heater Tester | 150,000 |
| Energy Savings with Advanced Building Materials | 150,000 |
| Recommended R-Levels - ZIP Program | 40,000 |
| CFC Foam Characterization | 70,000 |
| Foam Insulation Research | 75,000 |
| Development of Non-CFC Foam Insulations | 100,000 |
| Compact Vacuum Insulation | 125,000 |
| Evacuated Powder Panel Insulation | 150,000 |

# OFFICE OF BUILDING TECHNOLOGIES

## Office of Building Energy Research

The Office of Building Energy Research works to increase the energy efficiency of the buildings sector through performance of R&D on building systems and building equipment. In addition, 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

## Building Systems and Materials Division

The goal of this Division is to provide a scientific and technical basis (including model standards) for reducing the use of energy in residential and commercial buildings by 35 percent by the year 2000 from that used in 1975, while maintaining existing levels of human comfort, health and safety. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Building Materials Program seeks to develop new and improve existing insulating materials; to develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; to develop methods for measuring the thermal performance characteristics; and to provide technical assistance and advice to industry and the public. The DOE contact is Peter Scofield, (202) 586-9193.

## Materials Properties, Behavior, Characterization or Testing

1. Unguarded Thin Heater Tester - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact Tom Kollie, (615) 574-7463

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

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

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

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

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

   - Release version 2.0 of ZIP, the computer program that was used to calculate the recommended insulation levels.

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

   - Determine the sensitivity of variations in thermal conductivity and test specimen thickness in calibrating the R-matic and K-matic test apparatuses.

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

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

   - Develop foam thermal conductivity aging models.

6. Development of Non-CFC Foam Insulations - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact Tom Kollie, (615) 574-7463

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

   - Determine thermal properties and aging characteristics with laboratory testing.

   - Determine mechanical properties with application field testing.

7. Compact Vacuum Insulation - DOE Contact Peter Scofield, (202) 586-9193; SERI Contact Tom Potter, (303) 231-1083

   - Develop super insulation concepts using a hard vacuum in a panel formed by two metal sheets separated with spacers.

8. Evacuated Powder Panel Insulation - DOE Contact Peter Scofield, (202) 586-9193; ORNL Contact Tom Kollie, (615) 574-7463

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

# OFFICE OF INDUSTRIAL TECHNOLOGIES

| | FY 1990 |
|---|---|
| Office of Industrial Technologies - Grand Total | $17,668,000 |
| Office of Waste Reduction Technologies | $ 6,251,000 |
| Industrial Energy Efficiency Division | $ 2,788,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 1,168,000 |
| Advanced Heat Exchanger Material Technology Development | 445,000 |
| Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components | 200,000 |
| National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components | 63,000 |
| Ceramic Fiber Residue Measurement | 0 |
| Characterization of Beta Alumina for a Sodium Heat Engine Application | 460,000 |
| Device or Component Fabrication, Behavior or Testing | $ 1,620,000 |
| Ceramic Composite Heat Exchanger for the Chemical Industry | 0 |
| HiPHES System Design Study for Energy Production from Hazardous Wastes | 465,000 |
| HiPHES System Design for an Advanced Reformer | 800,000 |
| Ceramic Components for Stationary Gas Turbines in Cogeneration Service | 355,000 |

## OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Waste Reduction Technologies (Continued) | |
| Waste Material Management Division | $ 3,463,000 |
| Waste Utilization and Conversion | $ 2,463,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 2,463,000 |
| Wood Wastes to Adhesives | 545,000 |
| Waste Rubber-Polymer Composite | 417,000 |
| Zinc-Contaminated Steel Conversion | 150,000 |
| Silicon Oxide Recovery-Conversion | 851,000 |
| Waste Food Carbohydrates to Lactide Copolymer Plastics | 500,000 |
| Solar Materials Research | $ 1,000,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 1,000,000 |
| Materials Processing Using High Solar Photon Flux | 500,000 |
| Catalysts for Solar-Assisted Water Detoxification | 500,000 |
| Office of Industrial Processes | $11,417,000 |
| Improved Energy Productivity Division | $ 1,732,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 1,370,000 |
| Composite Cathode Material Development | 910,000 |
| Cerox Inert Anode Material | 460,000 |
| Lightweight Alumina Aggregate | 0 |
| High Temperature Fiber Insulation | 0 |

## OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Industrial Processes (Continued) | |
| Improved Energy Productivity Division (Continued) | |
| Materials Properties, Behavior, Characterization or Testing | $ 362,000 |
| Expand and Control Inert Electrode Cell Operating Conditions | 362,000 |
| Advanced Industrial Concepts Division | $ 9,685,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 3,750,000 |
| Aerogel Thermal Insulators | 300,000 |
| Chemical Vapor Deposition of Ceramic Composites | 850,000 |
| Thin-Wall Hollow Ceramic Spheres from Slurries | 150,000 |
| The Role of Inert Gas Entrapped in Rapidly Solidified Materials | 700,000 |
| Biobased Materials - Composites | 150,000 |
| Microwave-Driven Spray Drying | 350,000 |
| Magnetic Field Processing of Polymers | 350,000 |
| Electrochemical Synthesis of Conducting Polymers and Electrocatalysts | 800,000 |
| Polymers with Improved Surface Properties | 100,000 |
| Materials Structures and Composition | $ 3,400,000 |
| Modeling and Development of Ordered Intermetallic Alloys | 1,200,000 |
| Thermosetting Resins with Reversible Crosslinks | 150,000 |
| Biobased Materials - Packaging Plastics | 350,000 |
| Innovative Approaches to the Chemical Recycling of Plastics | 500,000 |
| Recycling of Sheet Molding Compounds | 0 |

## OFFICE OF INDUSTRIAL TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Industrial Processes (Continued) | |
| Advanced Industrial Concepts Division (Continued) | |
| Materials Structures and Composition (Continued) | |
| Laser Deposition of Thin Films for High Temperature Superconductors | 300,000 |
| Microwave Sintering and Joining of Advanced Ceramics (Zirconia-Toughened Alumina (ZTA) and Microwave Joining of Ceramics) | 600,000 |
| Biomimetic Thin Film Ceramic Coatings | 300,000 |
| Materials Properties, Characterization, Behavior or Testing | $ 1,435,000 |
| X-Ray Tomography for Ceramic Composites | 300,000 |
| Variable Insulation Concepts | 150,000 |
| Ordered Intermetallic Alloys for Corrosion Resistance (FeAl Development) | 185,000 |
| Characterization of SiC Whisker - $MoSi_2$ Composites for Elevated Temperature Applications | 800,000 |
| Device or Component Fabrication, Behavior or Testing | $ 900,000 |
| Chemically Specific Coatings | 350,000 |
| Development of High-Temperature Superconducting Magnets for High-Efficiency Motors and Power Electronics | 200,000 |
| Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets | 350,000 |
| Facilities | $ 200,000 |
| Multiple Frequency Microwave Energy Source and Furnace | 200,000 |

## OFFICE OF INDUSTRIAL TECHNOLOGIES

This Office supports a broad range of research, including long-term, high-risk, high pay-off R&D in the Advanced Industrial Concepts Division to shorter-term engineering in other divisions. Cost-shared research and development for industrial energy conservation technologies that offer large potential for saving scarce fuels is promoted. 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.

Office of Waste Reduction Technologies

Waste 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 office conducts research to develop advanced waste energy recovery technologies for the industrial sector.

Industrial Energy Efficiency Division

Materials Properties, Behavior, Characterization or Testing

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

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

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

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

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

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

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

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

13. Characterization of Beta Alumina for a Sodium Heat Engine Application - DOE Contact W. Parks, (202) 586-2093; ANL Contact R. Valentin, (708) 972-4493

- Assess state of the art in fabrication and quality control of beta alumina tubes.
- Assess alternative processing methods to improve commercial tubes.
- Model stress profiles during Sodium Heat Engine (SHE) operation.
- Determine stress limits for SHE components.

Device or Component Fabrication, Behavior or Testing

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

- Design and field test of heat exchanger for the chemical industry.
- Evaluation of composite systems in industry environment.

15. HiPHES System Design Study for Energy Production from Hazardous Wastes - DOE Contact S. Richlen, (202) 586-2078; Solar Turbines Incorporated Contact B. Harkins, (619) 544-5398

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

16. HiPHES System Design Study for an Advanced Reformer - DOE Contact S. Richlen, (202) 586-2078; Stone & Webster Engineering Corp. Contact J. Williams, (617) 589-7197

   - Development of preliminary design for high pressure heat exchange system (HiPHES) for an advanced convective reformer.
   - Identification of critical material and design problems.

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

   - Assess current ceramic components for stationary gas turbines for use in cogeneration systems.

Waste Material Management Division

Waste Utilization and Conversion

Industrial waste solid, liquid, and gaseous materials are waste because they have insufficient economic potential, thus they are landfilled or discharged to the environment. Economically useful wastes are termed by-products and constitute the objective of the Waste Utilization and Conversion program. Materials research can provide technologies to upgrade wastes or create new commodity materials so that wastes can have economic, i.e., added, value to become by-product materials of value to industry or commerce. The DOE contact is Jerome Collins (202) 586-2369.

Materials Preparation, Synthesis, Deposition, Growth or Forming

18. Wood Wastes to Adhesives - DOE Contact Alan Schroeder, (202) 586-1641; SERI Contact Helena Chum, 303 231-7249.

    - Convert wood wastes to adhesives and molding compounds via pyrolysis and blending with phenols.

    - Test resins for manufacture of insulation foam using limestone-CO2 as the blowing agent instead of CFCs.

19. Waste Rubber-Polymer Composite - DOE Contact Stuart Natof, (202) 586-2370; Air Products & Chemicals, Inc. Contact, Dr. Bernard Bauman, (215) 481-6053.

    - Convert finely ground waste tire rubber to chemically active feedstock to be used by plastics molders to reduce cost and/or improve properties of the molded parts.

    - Surface activation of waste tire rubber is achieved by blends of fluorine and chlorine.

20. Zinc-Contaminated Steel Conversion - DOE Contact Stuart Natof, (202) 586-2370; Argonne National Laboratory Contact, Edward J. Daniels, (708) 972-5279.

    - Single-step process removes zinc from galvanized scrap steel, results in clean steel and zinc for recycling.

    - Hot sodium hydroxide, anodic stripping/simultaneous electrowinning process.

21. Silicon Oxide Recovery-Conversion - DOE Contact Bruce Cranford, (202) 586-9496; Dow Corning Contact, James May, (517) 496-6047.

    - Develop closed silicon furnace to capture CO and SiO and return the SiO to the furnace as carbide feed.

    - Convert CO to methanol.

22. Waste Food Carbohydrates to Lactide Copolymer Plastics - DOE Contact Alan Schroeder, (202) 586-1641; Argonne National Laboratory Contact Dr. Robert Coleman, (708) 972-3268.

- Convert waste food industry carbohydrates to lactide copolymers.
- Develop applications as plastics which biodegrade to CO2 and water.

Solar Materials Research

The objective of solar materials research is to identify and develop viable materials processes that take advantage of the attributes of highly concentrated solar fluxes. Solar technology is able to supply concentrated radiant energy to surfaces with high efficiency and without many of the environmental liabilities of conventional power supplies.

Materials Preparation, Synthesis, Deposition, Growth or Forming

23. Materials Processing Using High Solar Photon Flux - DOE Contact Frank Wilkins, (202) 586-1684; SERI Contact Meir Carasso, (303) 231-1353

- Demonstrate diamond-like carbon film growth, and characterize processes for different substrate materials
- Demonstrate high-temperature superconducting film growth on different substrates.
- Modify alloys to obtain high corrosion resistance, hardness, and tribological properties by a variety of deposition and surface modification techniques.

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

- Characterize and improve the performance of metal oxide semiconductors for use as catalysts in solar photocatalytic oxidation of organic contaminants in water.

Office of Industrial Processes

This office 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.

Improved Energy Productivity Division

Materials Preparation, Synthesis, Deposition, Growth or Forming

25. 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 retrofit design in commercial cells to determine optimum factors influencing useful life and cell operation.

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

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

27. Lightweight Alumina Aggregate - DOE Contact M. J. McMonigle, (202) 586-2082; Alcoa Contact Al Pearson, (412) 337-2706

- Phase I was initiated to develop an alumina aggregate that would be 30 percent less dense, 80 percent of compression strength and not cost 20 percent more.

28. High Temperatures Fiber Insulation - DOE Contact M. J. McMonigle, (202) 586-2082; Manville Contact Phil Martin, (303) 478-5252

- Initiated Phase I of project to develop improved high performance refractory fibers with 200°C higher service temperature, lower shrinkage and greater microstructural stability.

Materials Properties, Behavior, Characterization or Testing

29. Expand and Control Inert Electrode Cell Operating Conditions - DOE Contact M. J. McMonigle, (202) 586-2082; PNL Contact Larry Morgan, (509) 375-3874

- Development of cermets for inert anodes.

- Phase I - characterize present high temperature insulation. Phase II - develop new insulating fiber that has increased service temperatures of 200°C.

Advanced Industrial Concepts Division

The mission of AICD is to support generic, long-term, high-risk applied R&D in those processes and technologies that underpin industrial unit operations. The AICD output provides a technology base to improve energy use efficiency and advance industrial capability to use alternative energy resources. Materials-related research in AICD is conducted in the Advanced Industrial Materials (AIM) Program. The AIM Program develops generic materials technologies brought to a stage for private industry or other government programs to advance further towards technology and engineering demonstration. The Program emphasizes materials as an enabling technology for industrial energy conservation and focuses on six areas: Structural Engineering Materials, Thermally Insulating Materials, Other Unique Materials (entirely superconducting ceramics at this time), Innovative Processing Technology, Lightweight and Biobased Materials (principally plastics recycling and environmental compatibility), and Materials System Reliability. The contact for the AIM Program is Marvin E. Gunn, (202) 586-5377.

Materials Preparation, Synthesis, Deposition, Growth or Forming

30. Aerogel Thermal Insulators - DOE Contact Marvin E. Gunn, (202) 586-5377; LBL Contact Arlon Hunt, (415) 486-5370

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

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

31. Chemical Vapor Deposition of Ceramic Composites - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contact Peter Angelini, (615) 574-4565; SNL-L Contact Mark Allendorf, (415) 294-2895; Thermoelectron Technologies Contact Peter Reagan, (617) 622-1347

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

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

32. Thin-Wall Hollow Ceramic Spheres from Slurries - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contact David L. McElroy, (615) 574-5976; Georgia Institute of Technology Contact J. Cochran, (404) 894-6104

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

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

33. The Role of Inert Gas Entrapped in Rapidly Solidified Materials - DOE Contact Marvin E. Gunn, (202) 586-5377; INEL Contact John Flinn, (208) 526-8127; SNLL Contact W. G. Wolfer, (415) 294-2307

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

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

34. Biobased Materials - Composites - DOE Contact Marvin E. Gunn, (202) 586-5377; SERI Contact Helena Chum, (303) 231-7249; University of Wisconsin Contact Ray Young, (608) 262-0873; U.S. Forest Products Laboratory Contact Roger Rowell, (608) 264-5816; University of Southern Mississippi Contact Lon Mathias, (601) 266-4868; Virginia Polytechnic Institute & State University Contact Wolfgang Glasser, (703) 231-4403

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

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

35. Microwave-Driven Spray Drying - DOE Contact Marvin E. Gunn, (202) 586-5377; LANL Contact F. Gac, (505) 667-5126

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

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

36. Magnetic Field Processing of Polymers - DOE Contact Marvin E. Gunn, (202) 586-5377, INEL Contact Alan Donaldson, (508) 526-2627/FTS 583-2627; LANL Contact Gerald Maestas, (505) 667-3973/FTS 843-3973

   - Exploratory studies of organic and inorganic polymers formed in magnetic fields to achieve unique structural and mechanical properties.

37. Electrochemical Synthesis of Conducting Polymers and Electrocatalysts - DOE Contact Marvin E. Gunn, (202) 586-5377; LANL Contacts Gerald Maestas, (505) 667-3973/FTS 843-3973 and S. Gottesfeld, (505) 667-0853

   - Growth of conducting polymer films on dielectric substrates for wide range of applications—battery electrodes, corrosion resistant coatings, sensors, and electric circuitry.

   - Development of ion-exchange techniques to fabricate carbon-supported platinum electrocatalyst particles less than 2nm in average diameter for fuel cell electrodes.

38. Polymers with Improved Surface Properties - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contact Peter Angelini, (615) 574-4565 and L. K. Mansur, (615) 574-4797

   - Development of innovative technology based on ion-beam or coating modification of polymer surfaces for improved wear, corrosion resistance, and strength.

Materials Structures and Composition

39. Modeling and Development of Ordered Intermetallic Alloys - DOE Contact Marvin E. Gunn, (202) 586-5377; LANL Contact A. D. Rollett, (505) 667-6133/FTS 843-6133; ORNL Contacts Peter Angelini, (615) 574-4565, C. T. Liu, (615) 574-4459, V. K. Sikka, (615) 574-5112, M. L. Santella, (615) 574-4805, and D. M. Nicholson, (615) 574-5873; Imperial College (U.K.) Contact D. G. Pettifor, 011-441-589-5111, ext. 5756

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

   - Micromechanical modeling of role of second phase on toughness of composite microstructures.

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

- Experimental verification of theoretical design.

40. Thermosetting Resins with Reversible Crosslinks - DOE Contact Marvin E. Gunn, (202) 586-5377; Polytechnic of New York Contact Giuliana Tesoro, (718) 643-5244

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

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

41. Biobased Materials - Packaging Plastics - DOE Contact Marvin E. Gunn, (202) 586-5377; SERI Contact Helena Chum, (303) 231-7249; Michigan Biotechnology Institute Contact Ramani Narayan, (517) 349-2970

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

42. Innovative Approaches to the Chemical Recycling of Plastics - DOE Contact Marvin E. Gunn, (202) 586-5377; SERI Contacts Helena Chum, (303) 231-7249 and Robert Evans, (303) 231-1384

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

43. Recycling of Sheet Molding Compounds - DOE Contact Marvin E. Gunn, (202) 586-5377; Stevens Institute of Technology Contacts K. E. Gonsalves, (201) 420-5779 and S. S. Stivala, (201) 420-5529

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

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

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

44. <u>Laser Deposition of Thin Films for High Temperature Superconductors</u> - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contacts Peter Angelini, (615) 574-4565, D. H. Lowndes, (615) 574-6306 and D. M. Kroeger, (615) 574-5155

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

45. <u>Microwave Sintering and Joining of Advanced Ceramics (Zirconia-Toughened Alumina (ZTA) and Microwave Joining of Ceramics)</u> - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contacts Peter Angelini, (615) 574-4565 and Ron Beatty, (615) 574-4536; Technology Assessment and Transfer, Inc. Contact R. Silberglitt, (301) 261-8373

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

46. <u>Biomimetic Thin Film Ceramic Coatings</u> - DOE Contact Marvin E. Gunn, (202) 586-5377; PNL Contact Gary McVay, (509) 375-3762

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

Materials Properties, Characterization, Behavior or Testing

47. X-Ray Tomography for Ceramic Composites - DOE Contact Marvin E. Gunn, (202) 586-5377; LLNL Contact J. Kinney, (415) 243-6669/FTS 532-6669

- Use of high intensity monochromatic X-rays at Stanford Synchrotron Radiation Laboratory to monitor chemical vapor infiltration of fiber-reinforced ceramic composites.

48. Variable Insulation Concepts - DOE Contact Marvin E. Gunn, (202) 586-5377; SERI Contact T. R. Penney, (303) 231-1754/FTS 327-1754

- Concept definition and exploratory R&D on modification of compact vacuum insulation to provide controlled and thermal insulation vs. transmission.

49. Ordered Intermetallic Alloys for Corrosion Resistance (FeAl Development) - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contacts Peter Angelini, (615) 574-4565 and C. T. Liu, (615) 574-4459

- Identify an FeAl composition with the best combination of room temperature ductility and corrosion resistance in oxidizing molten nitrate sale environments.
- Minor alloying additions to FeAl led to room temperature tensile ductility greater than 10 percent, (a five-fold increase over pure binary aluminide).
- FeAl compositions with excellent corrosion resistance in molten nitrate salts were also identified.

50. Characterization of SiC Whisker - $MoSi_2$ Composites for Elevated Temperature Applications - DOE Contact Marvin E. Gunn, (202) 586-5377; LANL Contact J. J. Petrovic, (505) 667-0125

- Develop SiC whisker-$MoSi_2$ matrix composites for elevated temperature structural applications in oxidizing environments.
- Solid solution alloying of the composite matrix yielded strengths at 1500° that were 8-10 times higher than pure $MoSi_2$, with retention of ductility and oxidation resistance.

Device or Component Fabrication, Behavior or Testing

51. Chemically Specific Coatings - DOE Contact Marvin E. Gunn, (202) 586-5377; SNLA Contact A. C. Frye, (505) 844-0787

- Develop a new class of chemical sensors for process monitors that will improve process energy efficiency.
- Use of sol-gel chemistry and surface modification techniques to develop oxide coatings with controlled pore sizes and tailored chemical properties.
- Obtain films with chemical selectivity based on both molecular size and chemical interactions.

52. Development of High-Temperature Superconducting Magnets for High-Efficiency Motors and Power Electronics - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contacts Peter Angelini, (615) 574-4565 and R. A. Hawsey, (615) 574-8057

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

53. Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets - DOE Contact Marvin E. Gunn, (202) 586-5377; PNL Contact Larry R. Pederson, (509) 375-2731; Boeing Aerospace Contact Thomas Luhman, (206) 234-2683

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

Facilities

54. Multiple Frequency Microwave Energy Source and Furnace - DOE Contact Marvin E. Gunn, (202) 586-5377; ORNL Contact Peter Angelini, (615) 574-4565/FTS 624-4565

- Design and construction of a furnace permitting sintering of ceramics with tailored microwave frequencies.

# OFFICE OF TRANSPORTATION TECHNOLOGIES

| | FY 1990 |
|---|---|
| Office of Transportation Technologies - Grand Total | $26,801,000 |
| Office of Transportation Materials | $15,036,000 |
| Office of Propulsion Systems | $11,765,000 |
| Advanced Propulsion Division | |
| Electric and Hybrid Propulsion Division | |
| Office of Alternative Fuels | $ 0 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 4,551,000 |
| High Temperature SX Silicon Carbide (WBS No. 1113) | 381,000 |
| Turbomilling of SiC (WBS No. 1116) | 110,000 |
| $TiB_2$ Whiskers (WBS No. 1117) | 0 |
| Powder Characterization (WBS No. 1118) | 110,000 |
| Sintered Silicon Nitride (WBS No. 1121) | 145,000 |
| $Si_3N_4$ Powder Synthesis (WBS No. 1123) | 0 |
| Microwave Sintering (WBS No. 1124) | 332,000 |
| Novel $Si_3N_4$ Process (WBS No. 1126) | 545,000 |
| Advanced Processing (WBS No. 1141) | 0 |
| Improved Processing (WBS No. 1142) | 690,000 |
| Advanced Processing (WBS No. 1143) | 0 |
| Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144) | 185,000 |
| Dispersion Toughened $Si_3N_4$ (WBS No. 1221) | 532,000 |
| Dispersion Toughened $Si_3N_4$ (WBS No. 1223) | 0 |
| Composite Development (WBS No. 1224) | 0 |
| Advanced Composites (WBS No. 1225) | 205,000 |
| Dispersion Toughened Oxide Composites (WBS No. 1231) | 360,000 |
| Transformation Toughened Ceramics Processing (WBS No. 1232) | 128,000 |
| Development of Toughened Ceramics (WBS No. 1237) | 0 |
| Low Expansion Ceramics (WBS No. 1242) | 253,000 |
| Vapor-Phase Lubrication System | 75,000 |

## OFFICE OF TRANSPORTATION TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Alternative Fuels (continued) | |
| Materials Preparation, Synthesis, Deposition, Growth or Forming (continued) | |
| Ion-Beam-Assisted Deposition of Lubricious Compounds | 200,000 |
| Ion Implantation/Mixing of Lubricious Oxides | 60,000 |
| HRRS Hard Coatings | 90,000 |
| Additives for High-Temperature Liquid Lubricants | 0 |
| IBAD of TiN and $Cr_2O_3$ | 75,000 |
| Self-Lubricating Ceramic Surfaces | 75,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 4,931,000 |
| Microstructural Modeling of Cracks (WBS No. 2111) | 82,000 |
| Adherence of Coatings (WBS No. 2212) | 22,000 |
| Dynamic Interfaces (WBS No. 2221) | 109,000 |
| Advanced Statistics Calculations (WBS No. 2313) | 0 |
| Microstructural Analysis (WBS No. 3111) | 50,000 |
| Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114) | 205,000 |
| Project Data Base (WBS No. 3117) | 105,000 |
| Characterization of Transformation-Toughened Ceramics (WBS No. 3211) | 100,000 |
| Fracture Behavior of Toughened Ceramics (WBS No. 3213) | 290,000 |
| Cyclic Fatigue of Toughened Ceramics (WBS No. 3214) | 286,000 |
| Tensile Stress Rupture Development (WBS No. 3215) | 321,000 |
| Rotor Materials Data Base (WBS No. 3216) | 315,000 |
| Toughened Ceramics Life Prediction (WBS No. 3217) | 327,000 |
| Ceramic Durability Evaluation AGT | 80,000 |
| Environmental Effects in Toughened Ceramics (WBS No. 3314) | 109,000 |
| LHR Diesel Coupon Tests (WBS No. 3315) | 150,000 |
| High Temperature Tensile Testing (WBS No. 3412) | 218,000 |
| Standard Tensile Test Development (WBS No. 3413) | 125,000 |

## OFFICE OF TRANSPORTATION TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Alternative Fuels (continued) | |
| Materials Properties, Behavior, Characterization or Testing (continued) | |
| Development of a Fracture Toughness Microprobe (WBS No. 0x15) | 72,000 |
| Non-Destructive Evaluation (WBS No. 3511) | 360,000 |
| Computed Tomography (WBS No. 3515) | 65,000 |
| Nuclear Magnetic Resonance Imaging (WBS No. 3516) | 136,000 |
| Powder Characterization (WBS No. 3517) | 100,000 |
| Spectroscopic Characterization (WBS No. 3518) | 76,000 |
| Surface Adsorption (WBS No. 3519) | 138,000 |
| Thermodynamics of Surfaces (WBS No. 3520) | 82,000 |
| Effect of a Lubricating Surface Layer on the Wear Mechanisms in Silicon Carbide-Whisker-Reinforced Silicon Nitride | 130,000 |
| IBAD Process Characterization | 250,000 |
| Wear-Machinability Relationships in Intermetallic Alloys | 153,000 |
| Thermochemical Surface-Damage Model for Ceramics | 50,000 |
| Additive Response of Base Oils | 50,000 |
| Advanced Materials/Lubricant Interactions | 135,000 |
| Liquid Lubricants for Advanced Heat Engines | 160,000 |
| Chemiluminescence of High-Temperature Additives | 80,000 |
| Technology Transfer and Management Coordination | $1,842,000 |
| Management and Coordination (WBS No. 111) | 825,000 |
| International Exchange Agreement (IEA) Annex II Management and Support (WBS No. 4115) | 708,000 |
| Standard Reference Materials (WBS No. 4116) | 309,000 |
| Device or Component Fabrication, Behavior or Testing | $15,477,000 |
| Ceramic Component Design Technology | 100,000 |
| Life Prediction Methodology (WBS No. 3222) | 763,000 |
| Life Prediction Methodology (WBS No. 3223) | 546,000 |
| Component Testing (WBS No. 3316) | 39,000 |

## OFFICE OF TRANSPORTATION TECHNOLOGIES (Continued)

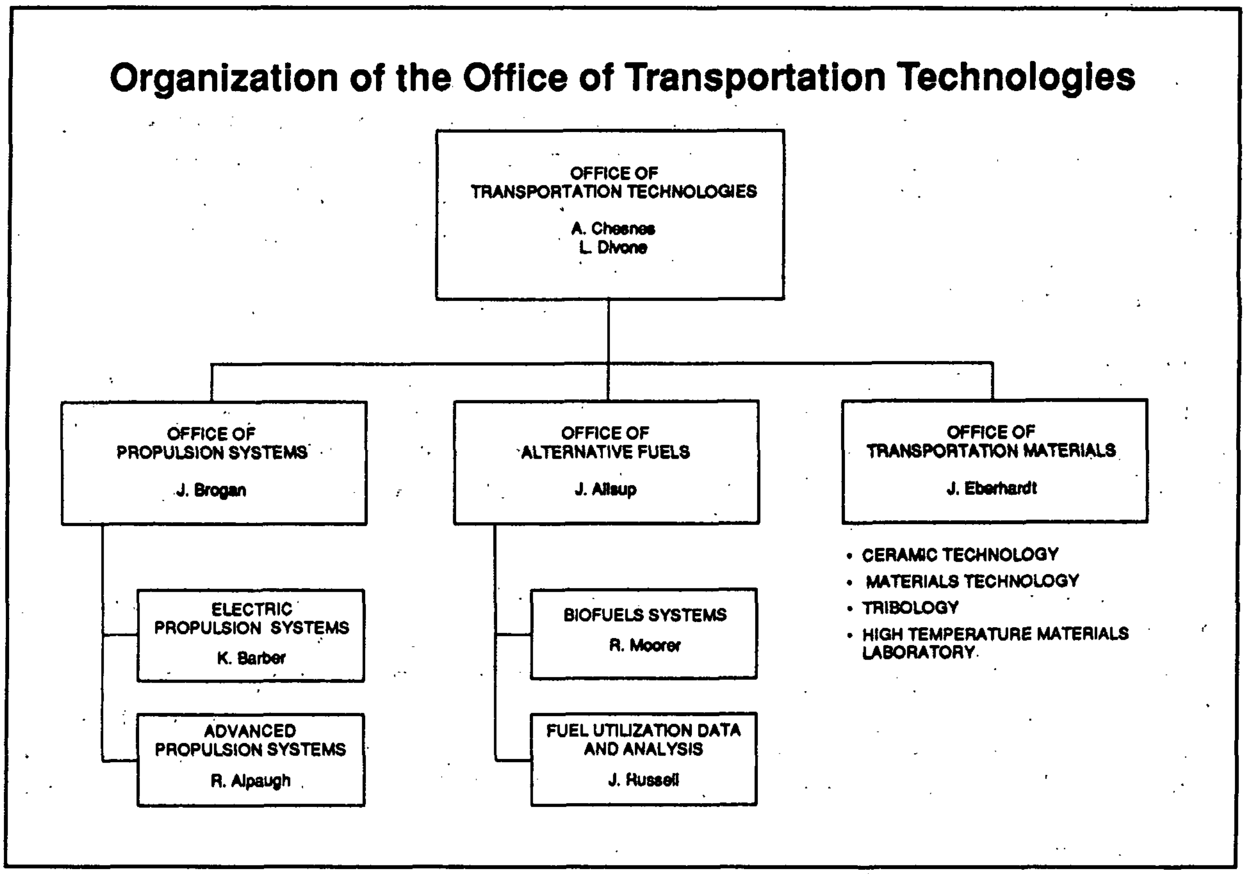
| | FY 1990 |
|---|---|
| Office of Alternative Fuels (continued) | |
| Device or Component Fabrication, Behavior or Testing (continued) | |
| Component Testing (WBS No. 3317) | 27,000 |
| Component Testing (WBS No. 3318) | 53,000 |
| Component Testing (WBS No. 3319) | 33,000 |
| Ceramic Component NDE Technology | 100,000 |
| Ceramic Mechanical Property Test Method Development (WBS No. 4121) | 200,000 |
| Advanced Coating Technology (WBS No. 1311) | 175,000 |
| Advanced Coating Technology AGT (WBS No. 1312) | 415,000 |
| Wear Resistant Coatings (WBS No. 1331) | 112,000 |
| Wear Resistant Coatings (WBS No. 1332) | 0 |
| Active Metal Brazing PSZ-Iron (WBS No. 1411) | 243,000 |
| Metal-Ceramic Joints AGT (WBS No. 1412) | 296,000 |
| Metal-Ceramic Joints AGT (WBS No. 1413) | 43,000 |
| Ceramic-Ceramic Joints AGT (WBS No. 1421) | 350,000 |
| Thick Thermal Barrier Coatings | 25,000 |
| Thick Thermal Barrier Coatings | 135,000 |
| Advanced Diesel Engine Component Development Project | 75,000 |
| Advanced Piston and Cylinder Component Development | 500,000 |
| Advanced Piston and Cylinder Component Development | 500,000 |
| High Temperature Solid Lubricant Coatings | 50,000 |
| Advanced Turbine Technology Applications Project (ATTAP, AGT-5) | 5,100,000 |
| Advanced Turbine Technology Applications Project (ATTAP, AGT-101) | 5,100,000 |
| IBAD Tribological Characterization | 260,000 |
| Energy-Efficient Gear-Lubrication Model | 50,000 |
| Lubrication Model | 75,000 |
| Wear Mechanism Modeling | 72,000 |

## OFFICE OF TRANSPORTATION TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Alternative Fuels (continued) | |
| Device or Component Fabrication, Behavior or Testing (continued) | |
| Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine | 0 |
| Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque | 0 |
| Surface Roughness Wear Model for Ceramics | 40,000 |
| Glassy-Carbon Materials for Severe Wear Environments | 0 |

## OFFICE OF TRANSPORTATION TECHNOLOGIES

The Office of Transportation Technologies has established a number of programs to conserve energy used for transportation and to shift transportation energy demand to nonpetroleum fuels. The Office of Transportation Technologies is divided into the Office of Propulsion Systems, Office of Alternative Fuels, and Office of Transportation Materials with each having program responsibility for specific technology and program areas. The organization of the Office of Transportation Technologies is shown in the following chart.




### Office of Transportation Materials

The Office of Transportation Materials conducts research programs to develop an industrial technology base in new transportation-related materials and materials processing in support of the Office of Transportation Technologies mission. Materials development activities consist of four main programmatic elements: Ceramic Technology (formerly Advanced Materials Development), Materials Technology (other than structural ceramics), Tribology, and the High Temperature Materials Laboratory.

The Ceramic Technology Program's objective is to establish an industrial technology base capable of providing reliable and cost-effective structural ceramics for applications to advanced heat engines. A balanced program is conducted in the areas of materials processing, design methodology, and data base and life prediction. A majority of the research is conducted by industry. The Ceramic Technology for Advanced Heat Engines (CTAHE) Project is managed by the Oak Ridge National Laboratory (ORNL). The DOE contact is Robert Schulz, (202) 586-8051.

The Materials Technology Program seeks to identify and resolve transportation materials problems other than those addressed under the Ceramic Technology Program. In the near-term, the program emphasizes improvements to available industry technology for materials problems in the fuel system, engine components and exhaust system of alternative-fueled (alcohol, natural gas) engines. For the mid- and long-term, the program will identify transportation-related materials requirements for electric propulsion, vehicle structure, and the transportation infrastructure. The DOE contact is James Eberhardt (Acting), (202) 586-5377.

The Tribology Program's objective is to provide a technology base for other transportation technology programs in the areas of lubrication, wear of lubricated solids, the friction and wear of ceramics, and tribological surface modifications and coatings. The Tribology Program is managed by Argonne National Laboratory (ANL). The DOE contact is James Eberhardt (Acting), (202) 586-5377.

The High Temperature Materials Laboratory (HTML) at Oak Ridge, Tennessee, is a research and user facility which supports Government and industry efforts in high temperature materials research and serves as a unique technology transfer vehicle through its user program. The HTML comprises six user centers: materials analysis, high temperature mechanical properties, high temperature x-ray diffraction, physical properties, ceramic specimen preparation, and residual stress measurements. The DOE contact is Ted Vojnovich, (202) 586-8060.

## Office of Propulsion Systems

The Office of Propulsion Systems is comprised of the Advanced Propulsion Division and the Electric and Hybrid Propulsion Division. Programs supported by this office are focused on developing, in cooperation with industry through cost-shared contracts, the technologies that will lead to the production and introduction of advanced vehicle propulsion systems and electric vehicles in the nation's transportation fleet.

Advanced Propulsion Division

The Advanced Propulsion Division has two major programs: Light Duty Engine Development focused on gas turbines through the Advanced Turbine Technology Applications Project (ATTAP) and Heavy Duty Engine Development focused on diesel engines through the Heavy Duty Transport Technology (HDTT) project. Materials activities supported by this Office and managed through the NASA Lewis Research Center for component and coating applications are included in this report. The DOE contacts are: Saunders Kramer, (202) 586-8000 for ATTAP and John Fairbanks, (202) 586-8012 for the HDTT project.

Electric and Hybrid Propulsion Division

The Electric and Hybrid Propulsion Division has three major programs: Battery Development, Fuel Cell Development, and Systems Development for electric vehicles. Materials work supported by this division is carried out by other DOE organizations and is thus not included in this section. The DOE contact is Pandit Patil, (202) 586-8055.

Office of Alternative Fuels

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

In this report, ceramic material (CTAHE) and component development (ATTAP, HDTT) projects are emphasized along with several tribology, lubricant development, and metals research projects. Not included in this report are biomass and other alternative fuel projects. Battery, fuel cell, semiconductor, electromagnetic, and other electrochemical material research that may support this office is sponsored by other DOE offices.

Materials Preparation, Synthesis, Deposition, Growth or Forming

55. High Temperature SX Silicon Carbide (WBS No. 1113) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Carborundum Contact Roger S. Storm, (716) 278-2544

- Establish a property database and analysis for the current best SX material.

- Optimize the processing conditions of that material via a designed experimental method.

- Optimize the second generation SX material with superior high temperature material properties.

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

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

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

    - The objective of this effort was to investigate the feasibility of developing a basic process to grow $TiB_2$ whiskers by the VLS method, characterize the whisker product, and evaluate the potential of the whiskers as reinforcements for high temperature ceramic composites and metal matrix composites.

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

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

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

    - Determine optimum sintering aid and time-temperature-pressure for sintered $Si_3N_4$ containing yttria/silica and small additions of $Mo_2C$.

    - Ceradyne, Inc., has been selected to carry out a scale-up and database generation and evaluation of a silicon nitride-yttria-silica base composition containing molybdenum carbide to be transitioned from AMTL to commercial prototype components in a test engine.

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

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

- To achieve major improvements in the quantitative understanding of how to produce sinterable Si$_3$N$_4$ powders having highly controlled particle size, shape, surface area, impurity content, and phase content.

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

- Identify those aspects of microwave processing of silicon nitride that might 1) accelerate densification, 2) permit sintering to high density using much lower levels of sintering aids, 3) lower the sintering temperature, or 4) produce unique microstructures.

62. Novel Si$_3$N$_4$ Process (WBS No. 1126) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact E. L. Long, Jr., (615) 574-5172; Sullivan Mining Corporation Contact Thomas M. Sullivan, (619) 692-1180

- Demonstrate scalability of the Sullivan™ Process for making silicon nitride, develop unique high- and low-temperature versions of the silicon nitride, determine the net-shape capability of the process, and characterize the microstructural, mechanical, tribological, and physical properties of the Sullivan™ Process silicon nitride.

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

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

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

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

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

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

66. Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact R. L. Beatty, (615) 574-4536; University of California Contact Fred F. Lange, (805) 961-8248

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

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

- Develop high toughness, high strength, refractory ceramic matrix composites which are amenable to low-cost, near-net-shape forming for application as structural components in automotive engines.
- Maximize the toughness in a high strength, high temperature SiC whisker/$Si_3N_4$ matrix material system that can be formed to shape by slip casting and densified by a method amenable to complex shape mass production.

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

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

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

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

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

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

- Tailor the whisker/matrix interface and determine the optimum whisker morphology for fracture toughness improvements for candidate $Si_3N_4$ matrix SiC whisker composites developed in Phase I.

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

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

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

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

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

- Develop zirconia toughened ceramics that exhibit high toughness and high strength at temperatures up to 1000 °C and can be fabricated by pressureless sintering to full density.

- Optimize the properties of two classes of transformation-toughened ceramics, Y-TZP ($Y_2O_3$) stabilized tetragonal zirconia polycrystals and Ce-ZTA ($CeO_2$-$ZrO_2$ toughened $Al_2O_3$), studied in Phase I.

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

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

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

- Increase the use temperature of three-layer composites by substituting $HfO_2$ for $ZrO_2$.

- Develop aqueous and nonaqueous slip casing techniques for three-layer composites in order to obtain better layer uniformity and to maximize residual compressive stress by optimizing the outer layer thickness.

- Superimpose temperature stresses on transformation-induced stresses in three-layer composites.

- Demonstrate improved thermal shock resistance and damage resistance in optimized composites.

74. Low Expansion Ceramics (WBS No. 1242) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact Victor J. Tennery, (615) 574-5123; Virginia Polytechnic Institute and State University Contact J. J. Brown, Jr., (703) 961-6777

- Develop an economic, isotropic, ultra-low thermal expansion ceramic material having stable properties above 1200°C.

- Continue investigation of two promising materials, a zircon (NZP) composition and a beta-eucryptite composition.

75. Vapor-Phase Lubrication System - DOE Contact J. J. Eberhardt, (202) 586-1694; The Pennsylvania State University Contact E. E. Klaus, (814) 865-2574

- Develop system for depositing vapor-phase lubricants and producing films onto metal and ceramic substrates for lubrication of heat engines and industrial machinery.

76. Ion-Beam-Assisted Deposition of Lubricious Compounds - DOE Contact J. J. Eberhardt, (202) 586-1694; ANL Contact Fred Nichols, (312) 972-8292

- Develop processes for ion-beam-enhanced deposition (IAD) of low friction lubricious coatings on engineered surfaces.

77. Ion Implantation/Mixing of Lubricious Oxides - DOE Contact J. J. Eberhardt, (202) 586-1694; ANL Contact Fred Nichols, (312) 972-8292

- Assess feasibility of forming a lubricious compound of boron in near-surface regions of metallic alloys and ceramics by ion implantation or ion-beam mixing.

78. HRRS Hard Coatings - DOE Contact J. J. Eberhardt, (202) 586-1694; BIRL Contact Raymond Fessler, (708) 491-4941

- Investigate the friction, wear and fatigue properties of nitride and carbide coatings of Ti, Zr and Hf deposited on steel and ceramic substrates by the high-rate reactive-sputtering process.

79. Additives for High-Temperature Liquid Lubricants - DOE Contact J. J. Eberhardt, (202) 586-1694; JPL Contact Emil Lawton, (818) 354-2982

- Evaluate precursor dinitrile compounds as lubricant additives for high temperature applications.

- Determine compatibility of proposed compounds with ceramic surfaces and lubricant additives that are commonly used in lubricating oils.

80. IBAD of TiN and $Cr_2O_3$ - DOE Contact J. J. Eberhardt, (202) 586-1694; NRL Contact Fred Smidt, (202) 767-4800

- Determine the mechanism by which IBAD produces beneficial modifications of tribological coatings on steel and silicon substrates.

- Establish the necessary correlations between IBAD processing and tribological properties such as friction, wear, and adhesion.

81. Self-Lubricating Ceramic Surfaces - DOE Contact J. J. Eberhardt, (202) 586-1694; Universal Energy Systems Contact Rabi Bhattacharya, (513) 426-6900

- Establish optimum conditions for ion implantation and ion-beam mixing of suitable additives into the surfaces of bulk $ZrO_2$, $Al_2O_3$, and hardened steel for obtaining self-lubricating low friction and wear characteristics.

Materials Properties, Behavior, Characterization or Testing

82. Microstructural Modeling of Cracks (WBS No. 2111) - 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

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

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

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

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

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

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

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

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

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

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

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

- Determine the microstructure of monolithic and composite ceramics and relate that microstructure to mechanical properties and material performance.

- Materials of interest are silicon carbides and silicon nitrides developed by U. S. manufacturers as part of this program and ATTAP.

- Relate microstructural observations to available mechanical test data.

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

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

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

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

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

- Conduct studies to determine the mechanical properties (creep, delayed failure, strength, and toughness) at elevated temperatures for toughened ceramics.

- Gain an understanding of how microstructure and composition influence the mechanical performance of these materials at elevated temperatures and the stability of these properties for extended periods of time.

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

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

- Establish a data base for design and analysis applications.

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

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

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

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

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

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

95. Ceramic Durability Evaluation AGT - DOE Contact Sauders B. Kramer, (202) 586-8000; NASA Contact Sunil Dutta, (216) 433-3282; Garrett Turbine Engine Contact Nancy Campbell, (602) 220-7006

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

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

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

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

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

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

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

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

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

100. <u>Development of a Fracture Toughness Microprobe (WBS No. 3415)</u> - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact W. C. Oliver, (615) 576-7245; Rice University Contact G. M. Pharr

- To develop a technique for measuring fracture toughness in thin films and small volumes on a spatially-resolved basis.

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

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

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

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

- Develop calibration methods for CT scanners for ceramic materials.

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

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

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

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

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

- *Identification, characterization, and modification of those aspects of the chemistry* and physics of a ceramic powder and of the powder/solvent interface that control processing.

- Development of standard methods of analysis for achieving the above.

- Development of procedures for writing specifications for ceramic powders that include any of the methods of analysis developed during this project.

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

- Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.

- Perform a thorough spectroscopic analysis and characterization of selected ceramic powders and/or whiskers in non-aqueous suspension.

106. Surface Adsorption (WBS No. 3519) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; Pennsylvania State University Contact J. H. Adair,(814) 863-0857

- Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.

- Conduct a study of the basic mechanisms of adsorption from non-aqueous solvents onto ceramic surfaces, and the modification of those surfaces to make them uniformly processable.

107. Thermodynamics of Surfaces (WBS No. 3520) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. A. Janney, (615) 574-4281; Rutgers University Contact D. J. Shanefield, (201) 932-2226

- Develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics.

- Determine the thermodynamic nature of the ceramic powder surface in non-aqueous powder suspension.

108. Effect of a Lubricating Surface Layer on the Wear Mechanisms in Silicon Carbide-Whisker-Reinforced Silicon Nitride - DOE Contact J. J. Eberhardt, (202) 586-1694; ORNL Contact Peter Blau, (615) 574-1514

- Study relationship between surface lubricating layers and wear mechanisms in the silicon carbide whisker-reinforced silicon nitride composites.

- Perform crystallographic modification of zirconia particles by altering the heat treatment process to improve the wear of zirconia-toughened composite over 400°C.

109. IBAD Process Characterization - DOE Contact J. J. Eberhardt, (202) 586-1694; ANL Contact Fred Nichols, (312) 972-8292

- Correlate film properties (adhesion, grain size, porosity, composition, etc.) with deposition parameters (ion type, ion-beam intensity, ion energy, deposition rate, substrate, etc.).

- Characterize wear scars of worn surfaces to determine wear mechanism(s).

110. Wear-Machinability Relationships in Intermetallic Alloys - DOE Contact J. J. Eberhardt, (202) 586-1694; ORNL Contact Peter Blau, (615) 574-1514

- Study machinability of new intermetallic alloys such as nickel and iron aluminides.
- Characterize high-speed sliding effects, high load effects, frictional heating, and other aspects of component fabrication processes.

111. Thermochemical Surface-Damage Model for Ceramics - DOE Contact J. J. Eberhardt, (202) 586-1694; Georgia Institute of Technology Contact Ward Winer, (404) 894-3270

- Investigate the effect of lubricant compositions on the wear of several advanced ceramics, including partially stabilized zirconia, silicon nitride, silicon carbide, sialon, and a superconducting ceramic.
- Develop surface-damage-control maps for various combinations of sliding speed and contact stress.

112. Additive Response of Base Oils - DOE Contact J. J. Eberhardt, (202) 586-1694; National Institute for Standards and Technology: Gaithersburg Contact Stephen Hsu, (301) 921-2113

- Separate lubricating base oils into their major fractions and subfractions, identify the molecular structures and chemical composition of the fractions and subfractions, and characterize the tribological performance of compound classes.
- Test additives with fractions to identify causes of synergistic and antagonistic effects.

113. Advanced Materials/Lubricant Interactions - DOE Contact J. J. Eberhardt, (202) 586-1694; National Institute for Standards and Technology: Gaithersburg Contact Stephen Hsu, (301) 921-2113

- Investigate fundamental mechanisms involved in interactions between synthetic base oils and additives, and ceramics such as silicon nitride, silicon carbide and alumina.
- Develop a test procedure for evaluating the performance of ceramic coatings for tribological applications in low heat rejection engines.

114. Liquid Lubricants for Advanced Heat Engines - DOE Contact J. J. Eberhardt, (202) 586-1694; National Institute for Standards and Technology: Gaithersburg Contact Stephen Hsu, (301) 921-2113

- Develop the necessary knowledge base for the selection and formulation of future lubricants for low heat rejection engines, including the base oil and the additives.

- Develop test methods to identify key structural and chemical requirements for super stable, high-temperature liquid lubricants.

115. Chemiluminescence of High-Temperature Additives - DOE Contact J. J. Eberhardt, (202) 586-1694; National Institute for Standards and Technology: Gaithersburg Contact Stephen Hsu, (301) 921-2113

- Explore use of chemiluminescence techniques for monitoring generation and control of lubricant oxidative stability, and the effects of catalysts and inhibitors.

Technology Transfer and Management Coordination

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

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

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

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

118. Standard Reference Materials (WBS No. 4116) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; National Institute of Standards and Technology (NIST) Contact S. Malghan, (301) 975-2000

- Develop standard reference material from the ceramic powder chosen by the U.S. consulting committee for the IEA agreement.
- Critical assessment and modeling of ceramic powder characterization methodology toward the establishment of an international basis for standard materials and methods for the evaluation of powders prior to processing.

Device or Component Fabrication, Behavior or Testing

119. Ceramic Component Design Technology - DOE Contact Saunders B. Kramer, (202) 586-8000; NASA Contact John Gyekenyesi, (216) 433-3210

- Develop probabilistic computer codes for ceramic component design.

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

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

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

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

122. Component Testing (WBS No. 3316) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Garrett Ceramic Components Division Contact M. V. Mitchell, (213) 618-6579

- Fabricate fuel pump push rod ends, valve spring seats, and tappet rollers from GS-44, a gas-pressure sintered silicon nitride.
- Test components in race car engines, analyze results, and prepare a report.

123. Component Testing (WBS No. 3317) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Carborundum Contact Roger S. Storm, (716) 278-2544

- Fabricate fuel pump push rod ends using Carborundum's sialon composition.
- Test components, analyze wear rate data, and prepare a report.

124. Component Testing (WBS No. 3318) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Detroit Diesel Allison Contact K. E. Weber, (313) 592-7224

- Inspect and test 100 domestically-produced silicon nitride cam-roller followers.
- Compare test results with results from foreign-produced cam-roller followers and prepare a report.

125. Component Testing (WBS No. 3319) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson, (615) 576-6832; Norton/TRW Contact T. G. Kalamasz, (603) 894-6775

- Fabricate two engine sets of intake and exhaust valves using a pressureless sintered silicon nitride material.
- Perform dynamics, performance, wear, and durability testing and compare with results from metal valves.

126. Ceramic Component NDE Technology - DOE Contact Saunders B. Kramer, (202) 586-8000; NASA Contact Alex Vary, (216) 433-6019

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

127. Ceramic Mechanical Property Test Method Development (WBS No. 4121) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. Ray Johnson (615) 576-6832; National Institute of Standards and Technology (NIST) Contact G. Quinn, (301) 975-5765

- Define and develop test methods in support of the Advanced Materials Development and the Advanced Turbine Technology Applications Programs.

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

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

129. Advanced Coating Technology AGT (WBS No. 1312) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact D. P. Stinton, (615) 574-4556; GTE Contact H. Rebenne, (617) 466-2528

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

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

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

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

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

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

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

133. Metal-Ceramic Joints AGT (WBS No. 1412) - DOE Contact Robert B. Schulz, (202) 586-8051; ORNL Contact M. L. Santella, (615) 574-4805; GTE Contact S. Kang, (617) 890-8460

- 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.

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

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

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

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

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

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

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

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

138. Advanced Diesel Engine Component Development Project - DOE Contact John W. Fairbanks, (202) 586-8066; NASA Contact Richard Barrows, (216) 433-3388; Detroit Diesel Corporation Contact Karen Weber, (313) 592-7224

- Develop advanced technology diesel engine components and integrate into test bed engine to demonstrate reduced emissions and improved fuel economy.
- Investigate use of advanced ceramic and metallic materials in structural, insulative, and tribological component applications.

139. Advanced Piston and Cylinder Component Development - DOE Contact John W. Fairbanks, (202) 586-8066 NASA Contact J. J. Notardonato, (216) 433-3908; Caterpillar Inc. Contact H. J. Larson, (309) 578-6549

- Develop advanced technology diesel engine components and integrate into test bed engine to demonstrate reduced emissions and improved fuel economy.
- Investigate use of advanced ceramic and metallic materials in structural, insulative, and tribological component applications.

140. Advanced Piston and Cylinder Component Development - DOE Contact John W. Fairbanks, (202) 586-8066; NASA Contact J. J. Notardonato, (216) 433-3908 Cummins Engine Contact D. H. Reichenbach, (812) 377-7041

- Develop advanced technology diesel engine components and integrate into test bed engine to demonstrate reduced emissions and improved fuel economy.
- Investigate use of advanced ceramic and metallic materials in structural, insulative and tribological component applications.

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

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

142. Advanced Turbine Technology Applications Project (ATTAP, AGT-5) - DOE Contact Saunders B. Kramer, (202) 586-8000; NASA Contact Paul Kerwin, (216) 433-3409; General Motors, Allison Gas Turbine Division, Contact Phil Haley, (317) 230-2272

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

143. Advanced Turbine Technology Applications Project (ATTAP, AGT-101) - DOE Contact Saunders B. Kramer, (202) 586-8000; NASA Contact Thomas N. Strom, (216) 433-3408; Garrett Turbine Engine Contact Jim Kidwell, (602) 220-3463

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

144. IBAD Tribological Characterization - DOE Contact J. J. Eberhardt, (202) 586-1694; ANL Contact Fred Nichols, (312) 972-8292

- Evaluate tribological performance of surface-modified substrates as a function of temperature, load, sliding velocity and sliding distance.

145. Energy-Efficient Gear-Lubrication Model - DOE Contact J. J. Eberhardt, (202) 586-1694; Northwestern University Contact Herbert Cheng, (312) 491-7062

- Model friction and wear in the partial elastohydrodynamic lubrication regime.

- Calculate power loss and wear loss in spur gears and perform experimental validation of friction and wear models.

146. Lubrication Model - DOE Contact J. J. Eberhardt, (202) 586-1694; National Institute for Standards and Technology: Gaithersburg Contact Stephen Hsu, (301) 921-2113

- Model the lubrication limits and predict wear life of simple materials under idealized contacting conditions.

- Develop a conceptual model to link all critical factors involving chemical and material-property control in the contact zone.

147. Wear Mechanism Modeling - DOE Contact J. J. Eberhardt, (202) 586-1694; Cambridge University Contact M. F. Ashby, 0-223-33-2-2622

- Use normalized coordinates to correlate, in a consistent manner, large and varied data base on steel-on-steel studies.

- Extend the treatment to include arbitrary combinations of wear/friction pairs with differing material properties.

148. Advanced Laser Fluorescence Measurements of Lubricant Film Behavior in a Diesel Engine - DOE Contact J. J. Eberhardt, (202) 586-1694; MIT Contact John Heywood, (617) 253-2243

- Establish a model of lubricant flow and residence time at top-ring reversal and in the top-ring zone of a typical top-tight-land-piston configuration similar to those used in prototype low heat rejection engines.

- Use advanced laser fluorescence to determine basic differences in oil-film characteristics of a production diesel engine with different lubricants and piston-ring designs.

149. Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque - DOE Contact J. J. Eberhardt, (202) 586-1694; Wayne State University Contact Naeim Henein, (313) 577-3887

- Develop techniques to evaluate instantaneous friction torque in an operating, reciprocating internal combustion engine.

- Conduct in-engine testing of surface-modified components using experimental test engine.

150. Surface Roughness Wear Model for Ceramics - DOE Contact J. J. Eberhardt, (202) 586-1694; SKF-MRC, Inc. Contact John McCool, (215) 889-1300

- Develop a personal computer-based software package (RUFFIAN) which predicts wear and load-bearing area, and aids in surface finish selection for ceramic bearings.

151. Glassy-Carbon Materials for Severe Wear Environments - DOE Contact J. J. Eberhardt, (202) 586-1694; Burton Technologies, Inc. Contact R. A. Burton, (919) 839-8287

- Evaluate tribological performance of a low-wear, vitreous-carbon material.
- Compare behavior of the glassy carbon to that of metals and ceramics subjected to the same severe conditions.

## OFFICE OF UTILITY TECHNOLOGIES

| | FY 1990 |
|---|---|
| Office of Utility Technologies - Grand Total | $33,847,788 |
| Office of Solar Energy Conversion | $19,250,000 |
| Solar Thermal and Biomass Power Division | $ 850,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 850,000 |
| Silver/Polymer Reflector Research | 850,000 |
| Photovoltaic Energy Technology Division | $18,400,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $13,500,000 |
| Amorphous Silicon for Solar Cells | 8,000,000 |
| 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 Renewable Energy Conversion | $ 599,700 |
| Geothermal Division | $ 599,700 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 285,000 |
| Materials for Non-Metallic Heat Exchangers | 85,000 |
| Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes | 200,000 |

## OFFICE OF UTILITY TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Renewable Energy Conversion (Continued) | |
| Geothermal Division (Continued) | |
| Materials Properties, Behavior, Characterization or Testing | $314,700 |
| Advanced High Temperature Geothermal Well Cements | 155,000 |
| Corrosion in Binary Geothermal Systems | 4,700 |
| Advanced High Temperature Chemical Systems for Lost Circulation Control | 95,000 |
| Corrosion Mitigation in Highly Acidic Steam Condensates | 60,000 |
| Office of Energy Management | $13,998,088 |
| Utility Systems Division | $ 125,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 125,000 |
| Gaseous Dielectric Decomposition, Detection, and Mitigation of $S_2F_{10}$ | 0 |
| Pre-Breakdown Events in Liquid Dielectrics | 125,000 |
| Advanced Utility Concepts Division | $13,873,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 137,000 |
| Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications | 137,000 |

## OFFICE OF UTILITY TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Energy Management (Continued) | |
| Advanced Utility Concepts Division (Continued) | |
| Materials Structure and Composition | $ 477,000 |
| Molten Salt Cell Research | 275,000 |
| New Battery Materials | 150,000 |
| Spectroscopic Studies of Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents | 52,000 |
| Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery | 0 |
| Materials Properties, Behavior, Characterization or Testing | $11,293,088 |
| High-Temperature Superconducting Materials Pilot Centers | 6,000,000 |
| Microfilamentary Superconducting Composite | 288,000 |
| Practical Superconductor Development for Electric Power Applications | 1,246,000 |
| Bulk Conductor Development/Device Technology Development | 527,000 |
| Thin Films Superconductors for Electric Power Applications | 384,000 |
| Bulk and Thin-Film Materials Process Research for High-Temperature Superconductor and Power Device Development | 767,000 |
| Development and Fabrication of High-Temperature Superconductors | 575,000 |
| Bulk Conductor Processing and Powder Development | 670,000 |

## OFFICE OF UTILITY TECHNOLOGIES (Continued)

| | FY 1990 |
|---|---|
| Office of Energy Management (Continued) | |
| Advanced Utility Concepts Division (Continued) | |
| Materials Properties, Behavior, Characterization or Testing (Continued) | |
| Materials Durability in the Zinc-Bromine System | 19,000 |
| Solid-Electrolyte Cell Research | 225,000 |
| Zinc Electrode Morphology in Acid Electrolytes | 100,000 |
| Zinc/Air Battery Development for Electric Vehicles | 149,000 |
| Polymeric Electrolytes for Ambient-Temperature Lithium Batteries | 47,000 |
| Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells | 0 |
| Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries | 88 |
| Advanced Chemistry and Materials for Fuel Cells | 100,000 |
| Electrocatalysts for Oxygen Reduction and Generation | 196,000 |
| Device or Component Fabrication, Behavior or Testing | $ 1,966,000 |
| Processing Methods of HTS Thin Films for Metal Tape Conductors | 384,000 |
| Proton-Exchange-Membrane Fuel Cells for Vehicles | 1,300,000 |
| Solid Polymer Electrolytes for Rechargeable Batteries | 97,000 |
| Advanced Membrane Development for the Zinc/Bromine System | 125,000 |
| Improved Chromium Platings for Sodium/Sulfur Containers | 60,000 |

## OFFICE OF UTILITY TECHNOLOGIES

The Office of Utility Technologies formulates, articulates, executes, and evaluates a national program of technology planning, research and development, and test and evaluation for utility technologies.

In addition, the Office is responsible for the development, execution, and evaluation of program specific technology transfer programs and activities to effect timely transfer of technology from Federal laboratories to energy production concerns, and facilitate informed decision-making within the energy utilization community.

Materials research within the Office of Utility Technologies is carried out by the Office of Solar Energy Conversion, the Office of Renewable Energy Conversion and the Office of Energy Management.

### Office of Solar Energy Conversion

The mission of the Office of Solar Energy Conversion is to provide overall direction, interpret policy objectives, and establish management procedures for a balanced program of technology planning, research, development, test, analysis, evaluation, and communication that will foster the establishment of solar energy supply options for use by utilities and allied industries and institutions.

The Office represents, as the national programmatic expert, the photovoltaic and solar thermal and biomass power—technologies in the formulation and execution of national energy policies and programs. The Office is responsible for the establishment of program balance and priorities among subordinate Divisions.

### Solar Thermal and Biomass Power Division

The mission of the Solar Thermal and Biomass Power Division is to plan and manage a balanced program for technology research, development, testing and evaluation which will foster the establishment of solar thermal energy and biomass power technology supply options.

The Division serves as the national federal technical expert for the purpose of formulating and executing national energy policies and programs relating to solar thermal and biomass power technologies.

Materials Preparation, Synthesis, Deposition, Growth or Forming

152. Silver/Polymer Reflector Research - DOE Contact Martin Scheve, (202) 586-8110; SERI Contact Gary Jorgenson, (303) 231-1226

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

Photovoltaic Energy Technology Division

The mission of the Photovoltaic Technology Division is to plan and mange a balanced program for technology research, development, testing and evaluation which will foster the establishment of photovoltaic energy technology supply options.

The Division serves as the national federal technical expert for the purpose of formulating and executing national energy policies and programs relating to photovoltaic technology.

Materials Preparation, Synthesis, Deposition, Growth or Forming

153. Amorphous Silicon for Solar Cells - DOE Contact Morton B. Prince, (202) 586-1725; SERI Contact Richard Crandall, (303) 231-1913

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

154. 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.

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

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

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

Materials Properties, Behavior, Characterization or Testing

156. 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

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

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

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

- Study of fundamental problems of ribbon growth.

Office of Renewable Energy Conversion

The mission of the Office of Renewable Energy Conversion is to provide overall direction, interpret policy objectives, and establish management procedures for a balanced program of technology planning, research, development, test, analysis, evaluation, and communication that will foster the establishment of renewable or alternate energy supply options for use by utilities and allied industries and institutions.

The Office represents, as the national programmatic expert, the wind, hydropower, oceans and geothermal technologies in the formulation and execution of national energy policies and programs. The Office is responsible for the establishment of program balance and priorities among subordinate Divisions.

Geothermal Division

The mission of the Geothermal Division is to plan and manage a balanced program for technology research, development, testing and evaluation which will foster the establishment of geothermal technology supply options.

The Division serves as the national federal technical expert for the purpose of formulating and executing national energy polices and programs relating to geothermal technology.

Materials Preparation, Synthesis, Deposition, Growth or Forming

158. Materials for Non-Metallic Heat Exchangers - DOE Contact R. LaSala, (202) 586-4198; BNL Contact L. E. Kukacka, (516) 282-3065

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

159. Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes - DOE Contact G. J. Hooper, (202) 586-1146; BNL Contact E. T. Premuzic, (516) 282-2893

- Analyses of biochemical techniques for concentrating and subsequent removal of toxic metals from waste.

- Establishment of optimum conditions for microorganism-metal interactions.

Materials Properties, Behavior, Characterization or Testing

160. Advanced High Temperature Geothermal Well Cements - DOE Contact R. LaSala, (202) 586-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- Development of lightweight, $CO_2$ resistant high temperature well cements.
- Characterization of well completion materials under placement and downhole environmental conditions.

161. Corrosion in Binary Geothermal Systems - DOE Contact R. LaSala, (202) 586-4198; BNL Contact D. van Rooyen, (516) 282-4050

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

162. Advanced High Temperature Chemical Systems for Lost Circulation Control - DOE Contact R. LaSala, (202) 586-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- Chemical and mechanical property characterization of advanced inorganic chemical systems added to bentonite-based drilling fluids.
- Field characterization of lined downhole and above ground equipment.

163. Corrosion Mitigation in Highly Acidic Steam Condensates - DOE Contact R. LaSala, (202) 586-4198; BNL Contact L. E. Kukacka, (516) 282-3065

- Development of high temperature acid resistance polymer matrix composite liner formulations.
- Field characterization of lined downhole and above ground equipment.

Office of Energy Management

The mission of the Office of Energy Management is to provide federal leadership for the research and development of new technologies and processes that promote efficiency, reliability, and flexibility in the nation's utility energy delivery systems. The Office manages programs in utility systems and advanced utility concepts and is responsible for leading R&D centers consistent with DOE and CE policies, establishing 5-year program goals, consolidating organizational units to focus resources, and pursuing leveraging opportunities with industry, utilities, and other government agencies by providing technology transfer assistance, encouraging Cooperative Research and Development Agreement (CRADA) establishment, and implementing cost-shared research programs.

Utility Systems Division

The Utility Systems Division supports research and development directed toward solving mid- to long-term problems in electric energy transmission and distribution and promotes the development and integration of new materials, advanced controls, and new design concepts into the utility network. The program supports research activities in the following areas: Integrated Resources Planning, Electric Field Effects, Transmission and Distribution Technologies, and District Heating and Cooling.

Materials Properties, Behavior, Characterization or Testing

164. Gaseous Dielectric Decomposition, Detection, and Mitigation of $S_2F_{10}$ - DOE Contact R. Eaton, (202) 586-1506; Oak Ridge National Laboratory Contact D. R. James, (615) 574-0266

   - Develop detection techniques permitting sensitive detection of $S_2F_{10}$ gas in dielectrics, and determining toxicity of $S_2F_{10}$ in $SF_6$ environments.

165. Pre-Breakdown Events in Liquid Dielectrics - DOE Contact R. Eaton, (202) 586-1506; University of Tennessee Contact M. O. Pace, (615) 974-5419

   - Gain a better understanding of pre-breakdown events in liquid dielectrics to improve liquid insulated power equipment.

Advanced Utility Concepts Division

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

Materials Preparation, Synthesis, Deposition, Growth or Forming

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

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

Materials Structure and Composition

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

- Investigate high-temperature immobilized electrolyte materials to improve the Li-alloy/metal disulfide cell.

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

- Characterize high-sodium-activity alloys and low-melting-point molten salts for sodium metal chloride cells.

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

- Prepare and characterize submonolayer deposits of alkali and alkaline earth metals on metal surfaces and develop understanding of passive surface layers in rechargeable alkali batteries.

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

- Investigate lithium and zinc electrode surface in solutions using *in situ* Raman spectroscopy.

Materials Properties, Behavior, Characterization or Testing

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

- Aggressively continue HTS research and development by encouraging technology transfer between laboratories and industry through pilot centers.

172. Microfilamentary Superconducting Composite - DOE Contact R. Eaton, (202) 586-1506; Ames Laboratory Contact D. K. Finnemore, (515) 294-3455

- Develop materials processing technique to make stabilized microfilamentary superconducting wires for magnets operating at 35K.

173. Practical Superconductor Development for Electric Power Applications - DOE Contact R. Eaton, (202) 586-1506; Argonne National Laboratory Contact R. Poeppel, (708) 972-5118

- Develop methods to fabricate HTS long wires and tapes, and develop devices such as electrical contacts, coils, and windings.

174. Bulk Conductor Development/Device Technology Development - DOE Contact R. Eaton, (202) 586-1506; Brookhaven National Laboratory Contact D. Welch, (516) 282-3517

- Develop composite conductor fabrication methods for large-scale production for electrical power systems applications.

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

- Identify and develop thin-film fabrication techniques suitable for manufacture of high-current carrying long wires and tapes for use in making components of electric power system devices.

176. Bulk and Thin-Film Materials Process Research for High-Temperature Superconductor and Power Device Development - DOE Contact R. Eaton, (202) 586-1506; Sandia National Laboratory Contact T. Bickel, (505) 844-2392

- Develop bulk and thin-film high-temperature superconducting materials and processes with properties suitable for use in electric energy systems.

177. Development and Fabrication of High-Temperature Superconductors - DOE Contact R. Eaton, (202) 586-1506; Los Alamos National Laboratory Contact D. Peterson, (505) 667-3973

- Fabricate a bulk superconductor with critical current density of $10^4$ A/cm$^2$ at 35K and 2T using efficient and reproducible approaches enabling fabrication of pieces appropriate for use in power applications.

178. Bulk Conductor Processing and Powder Development - DOE Contract R. Eaton, (202) 586-1506; Oak Ridge National Laboratory Contact D. Kroeger, (615) 574-5177

- Develop materials information and processing techniques applicable to production of high-$T_c$ oxide superconductors in bulk form with high current density.

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

- Improve chemical durability of materials in zinc/bromine battery environments.

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

- Develop glass-to-header seals that are mechanically stable and provide hermetic seals for use in sodium/sulfur cells.

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

- Study zinc electrode morphology in acidic zinc chloride and zinc bromine electrolytes to provide the fundamental information needed to improve the design and performance of zinc/halogen batteries.

182. Zinc/Air Battery Development for Electric Vehicles - DOE Contact A. Landgrebe, (202) 586-1483; Metal Air Technology Systems International Contact R. Putt, (404) 876-8203

- Investigate electrode structure and coating techniques for use in zinc/air battery for electric vehicles.

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

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

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

- Develop high-performance solid-polymer-electrolyte rechargeable cells for use in electric vehicles or utility load-leveling systems.

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

- Investigate the passivation behavior of iron in anhydrous propylene carbonate containing 0.5M $LiClO_4$.

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

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

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

- Examine monolayers of absorbed iron and tetrasulfonated phthalocyanine on nitrogen-containing polymers using *ex situ* and *in situ* Fourier transform infrared reflectance absorption spectroscopy.

Device or Component Fabrication, Behavior or Testing

188. Processing Methods of HTS Thin Films for Metal Tape Conductors - DOE Contact R. Eaton, (202) 586-1506; Lawrence Berkeley Laboratory Contact N. E. Phillips, (415) 486-4896

- Investigate methods for producing thin films of high-$T_c$ superconductors with appropriate substrate, buffer, and passivating materials to provide a basis for the fabrication of practical tape conductors.

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

- Research proton-exchange-membrane fuel cells, including developing batter electrodes and membranes, and measuring operating characteristics to determine conditions providing optimum performance.

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

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

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

- Select and evaluate chemical pretreatment techniques for use on the silica-microporous polyethylene separators used in zinc/bromine battery technology.

192. Improved Chromium Platings for Sodium/Sulfur Containers - DOE Contact A. Landgrebe, (202) 586-1483; Sandia National Laboratory Contact J. W. Braithwaite, (505) 844-7749

- Identify techniques to improve the quality and efficiency of plating chromium onto the inside of sodium-sulfur containers.

## OFFICE OF ENERGY RESEARCH

| | FY 1990 |
|---|---|
| Office of Energy Research - Grand Total | $227,437,657 |
| Office of Basic Energy Sciences | $205,653,806 |
| Division of Materials Sciences | $198,400,000 |
| Division of Engineering and Geosciences | $ 6,481,806 |
| Materials Properties, Behavior, Characterization or Testing | $ 6,358,806 |
| New Ultrasonic Imaging and Measurement Techniques for NDE | 254,388 |
| Bounds on Dynamic Plastic Deformation | 127,194 |
| Continuous Damage Theory | 53,000 |
| Transport in Porous/Disordered Media | 66,650 |
| Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding | 47,804 |
| A Micromechanical Viscoplastic Strain-Strain Model with Grain Boundary Sliding | 46,048 |
| In-Flight Measurement of the Temperature of Small, High Velocity Particles | 182,137 |
| Plasma-Particle Interaction | 568,805 |
| Modeling of Thermal Plasma Processes | 0 |
| Nondestructive Evaluation of Superconductors | 177,371 |
| Intelligent Control of Thermal Processes | 480,000 |
| Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws | 385,706 |
| Heat Transfer to Aqueous Polymer Solutions | 70,144 |
| Pulse Propagation in Inhomogeneous Optical Fibers | 76,091 |
| High-Temperature Gas-Particle Reactions | 123,110 |
| Mathematical Modeling of Transport Phenomena in Plasma Systems | 92,806 |
| Multivariable Control of the Gas-Metal Arc Welding Process | 152,467 |
| Metal Transfer in Gas-Metal Arc Welding | 124,057 |
| Modeling and Analysis of Surface Cracks | 188,453 |
| Thermal Plasma Processing of Materials | 129,723 |
| Thermophysical Property Measurements in Fluid Mixtures | 509,486 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| Division of Engineering and Geosciences (continued) | |
| Materials Properties, Behavior, Characterization or Testing (continued) | |
| Low Resistivity Ohmic Contacts Between Semiconductors and High-Tc Superconductors | 94,700 |
| Transport Properties of Disordered Porous Media from the Microstructure | 91,859 |
| Effects of Crack Geometry and Near-Crack Material Behavior on Scattering of Ultrasonic Waves for QNDE Applications | 80,921 |
| Inelastic Deformation and Damage at High Temperature | 122,541 |
| Flux Flow, Pinning, and Resistive Behavior in Superconducting Networks | 63,594 |
| Energy Changes in Transforming Solids | 161,000 |
| Nondestructive Testing | 252,549 |
| Effective Elastic Properties of Cracked Solids | 53,987 |
| Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes | 175,217 |
| Thermodynamics of High Temperature Brines | 98,600 |
| Studies of the Interactions Between Mineral Surfaces and Ions in Solutions | 88,740 |
| Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions | 147,900 |
| Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures | 108,460 |
| Solubilities of Calcite and Dolomite in Hydrothermal Solutions | 98,600 |
| Salinity Effects on Oxygen and Hydrogen Isotope Partitioning Between Geothermal Brines and Other Phases at Elevated Temperatures | 63,104 |
| Advective-Diffusive/Dispersive Transport of Chemically Reacting Species in Hydrothermal Systems | 120,000 |
| Rock Mechanics: Thermal Stress Microfracturing of Crystalline and Sedimentary Rocks | 108,460 |
| Diffusion of Silicate Materials | 88,740 |
| Rheology of Melts | 167,620 |
| Microcrack Growth in Crystalline Rock | 69,020 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | | FY 1990 |
|---|---|---|
| Division of Engineering and Geosciences (continued) | | |
| Materials Properties, Behavior, Characterization or Testing (continued) | | |
| Experimental Database and Predictive Theories for Thermodynamic Properties of Aqueous Solutions | | 55,943 |
| Physical Characterization of Magma Samples | | 0 |
| Investigations of Ultrasonic Surface Wave Interaction with Porous Saturated Rocks | | 54,000 |
| Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage | | 59,811 |
| PVTX Properties of Fluid Systems: NaCl-$CaCl_2$-$H_2O$ | | 78,000 |
| Materials Structure and Composition | $ | 123,000 |
| Silicate Thermochemistry | | 123,000 |
| Division of Advanced Energy Projects | $ | 772,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ | 525,000 |
| Gas Jet Deposition of Metallic, Semiconducting and Insulating Films | | 150,000 |
| Growth of High Tc Superconducting Fibers Using a Miniaturized Laser-Heated Float Zone Process | | 375,000 |
| Materials Properties, Behavior, Characterization or Testing | $ | 247,000 |
| Production of Fuels and Chemicals From Methane | | 247,000 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| Small Business Innovation Research Program | $21,783,851* |
| Materials Preparation, Synthesis, Deposition, Growth, or Forming | $ 9,022,090 |
| Phase I Projects: | |
| Low Cost Iron Microparticles for Slurry Catalyzed Coal Liquefaction | 49,994 |
| Improved Enhanced Oil Recovery Processes Using Novel Synthetic Copolymers Containing Large Amounts of Acrylamide | 47,890 |
| Single Crystal Molybdenum Mirrors for High Power Vacuum Ultraviolet and X-Ray Radiation | 49,827 |
| Ultrafine Grained Molybdenum Silicide with Ultrafine Hafnium Carbide Dispersoids for Improved Superplastic Formability | 50,000 |
| A Large Area, Position Sensitive Detector for Synchrotron X-Ray Diffraction | 50,000 |
| Gas Jet Injection of Clusters into Liquids | 49,642 |
| Silicon Carbide Coatings for Synchrotron Optics | 49,966 |
| Innovative Mirror Technology for X-Ray Reflective Optics | 47,836 |
| A Method of Producing Carbon Clusters | 48,921 |
| Strength, Reliability, and Surface Hardness Improvement of Structural Ceramics Through Ion Implantations | 49,983 |
| Thin Film Tungsten Diselenide Photoelectrodes | 50,000 |
| Development of High-Performance Chemically Resistant Composite Membranes | 50,000 |
| Molecular Recognition in Metal Ion Sensors | 50,000 |
| Ultrathin Metal Membranes | 49,974 |
| Development of Oxidation-Resistant Mosaic Membranes with Enhanced Transport Properties | 49,999 |
| A Diamond X-Ray Detector | 50,000 |

*Includes 78 new Phase I and 27 new Phase II projects initiated in FY 1990 and 9 Phase II projects initiated in FY 1989. The funding shown for each Phase II project is the total allocated for the duration of the project (up to two years).

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| **Materials Preparation, Synthesis, Deposition, Growth or Forming (continued)** | |
| Phase I Projects: (continued) | |
| Changes in Niobium Tin Conductors Made by the Internal Tin Method to Improve Magnet Performance | 49,975 |
| Alternative Fabrication Processes for Ultrafine Filament, Metal Matrix Microcomposites | 49,978 |
| A Novel Carbon First Wall Material | 49,827 |
| Development of Radiation-Resistant Copper Matrix Composites | 50,000 |
| Initial Exploration of Amorphous and Polycrystalline Silicon Thin Film Transistors as Preamplifiers for Particle Detector Applications | 49,945 |
| Development of New Radiation Resistant Fluors with Large Stokes Shift and High Quantum Efficiency | 50,000 |
| Low Cost, Large Area Epitaxial Silicon Detectors for Sampling Calorimeters | 49,950 |
| Economic Low Loss Niobium Tin for Pulsed Field Applications, Made by a Modified Internal Tin Process | 49,951 |
| Development of Practical Multifilamentary Superconductors Using Chevrel Phase Materials for Magnet Applications at More Than 20 Tessla | 49,971 |
| A Thallium-Barium-Calcium-Copper Oxide, Thin Film, Superconducting Radio Frequency Cavity | 49,999 |
| Superconducting Radio Frequency Cavity Coatings by Metallorganic Chemical Vapor Deposition | 49,907 |
| New Scintillator Materials | 49,940 |
| Scintillating Optical Fibers of Barium Fluoride for Nuclear Instrumentation | 49,921 |
| A New Semiconductor Photosensor for Scintillation Spectroscopy | 50,000 |
| Highly Parallel, High Bandwidth, Optical Holographic Analog-to-Digital Convertors | 49,991 |
| Electrodeposition of Silicon Films from Liquid-Metal Solutions for Photovoltaic Applications | 50,000 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| Materials Preparation, Synthesis, Deposition, Growth or Forming (continued) | |
| Phase I Projects: (continued) | |
| Magnetically Enhanced Plasma Deposition of Intrinsic Hydrogenated Amorphous Silicon Layers in Roll-to-Roll Systems | 49,981 |
| Thermally Conductive, Solid-State Thermal Energy Storage Materials With High Latent Heats | 50,000 |
| Innovative Methods for the Production of Polymers from Biobased Materials | 49,932 |
| Development of a Low Cost, Continuous, Elastic, Reservoir Process to Produce Composite Sandwich Panels | 50,000 |
| A Novel Precursor Yarn for Advanced Automotive Composite Structures | 49,798 |
| Structural Tannin-Based Lumber End-Joint Adhesives for Existing Product Lines | 47,200 |
| Polypropylene Composites Reinforced with Biobased Graft Polymer | 48,900 |
| Property-Enhanced Composites from Lignocellulosic Fibers | 45,227 |
| Fiber Optic Bus-Organized Systems for Sensor Data Acquisition and Validation | 49,220 |
| Phase II Projects: (First Year) | |
| Low Temperature Processing of High $T_c$ Superconductor Films for Integration of Detector Arrays with Silicon Circuitry | 499,782 |
| Improved Thin Film Multilayer Coatings for Thermal Neutron Guides | 500,000 |
| Development of a Fabrication Process which Demonstrates the Commercial Feasibility of Supermirror Coatings for Neutron Guides | 500,000 |
| Thallium Bromoiodide Detectors for Scintillation Spectroscopy | 500,000 |
| Development of Internal Tin $Nb_3Sn$ Conductors by Novel Manufacturing Techniques | 499,798 |
| Ultrafine Filament NbTi Superconductors | 499,950 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| **Materials Preparation, Synthesis, Deposition, Growth, or Forming** (continued) | |
| **Phase II Projects:** (First Year) (continued) | |
| A Radiation Resistant Cryogenic Temperature Sensor for the 4K to 80K Range | 499,454 |
| Highly Conducting/Irradiation Resistant Carbon-Carbon Composites for Fusion Devices | 499,059 |
| Copper Infiltrated Graphite for Improved Brazed Joints | 500,000 |
| Recyclable Molds for Casting Nuclear Fuel | 499,955 |
| Ceramic Composite Materials for Pyrometallurgical Reprocessing | 500,000 |
| Corrosion Resistant Catalyst Supports for Phosphoric Acid Fuel Cells | 499,737 |
| Corrosion Resistant Carbons for Air Cathodes in Phosphoric Acid Fuel Cells | 490,910 |
| High Rate Polymer Electrolyte-Based Rechargeable Lithium Batteries | 499,800 |
| Highly Conductive Polymer Electrolytes | 499,991 |
| Polymer Solid Electrolytes with Specific Cation Conduction | 499,373 |
| **Phase II Projects:** (Second Year) | |
| A Mass Production Facility for Plastic Scintillating Optical Fibers with Radiation-Hardened Properties for the Superconducting Super Collider | 500,000 |
| A Ceramic Membrane for Gas Separations | 492,660 |
| Radiation-Modified Pyroelectric Conversion Materials | 499,972 |
| The Development of Multifilamentary Superconducting Composites | 500,000 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| **Materials Properties, Behavior, Characterization or Testing** | |
| **Phase I Projects:** | |
| Development of Computer-Controlled Scanning Electron Microscopy Techniques for Predicting the Cleaning Behavior of Coal | 49,846 |
| Utilization of Fluidized Bed Residuals for Producing Synthetic Aggregate by Vacuum Extrusion | 49,428 |
| An Evaluation in a Simulated Fluidized-Bed Combustion Environment of Erosion Resistance of Coatings Applied Using a Hypersonic Spray Process | 50,000 |
| A Holographic and Reflection X-Ray Laser Microscope for Lithographic Inspection | 49,937 |
| Subsurface Gamma Ray Backscatter Scanning Microscopy | 49,938 |
| Three-Dimensional Inspection of First Wall Surfaces for the Compact Ignition Tokamak | 46,092 |
| A Technique for Measuring Diffusion of Hydrogen Isotopes in Oxides | 50,000 |
| Failure Criteria for Drawing and Extrusion of Trimetal Superconducting Composite Wire | 50,000 |
| Piezoelectrically Driven Micropositioners for Rotation at Normal and Cryogenic Temperature in High Magnetic Fields | 48,529 |
| Nondestructive Evaluation of Superconducting Magnet Wire Using a Scanning Acoustic Pulse Spectroscope | 50,000 |
| A Novel, Robust, High Repetition, High Brightness Cathode | 49,999 |
| An All-Solid-State Titanium-Doped Sapphire Laser Source for Production of Polarized Electrons | 49,789 |
| In-Situ Diagnostic Technique for Process Monitoring and Control of the Plasma Deposition of Amorphous Hydrogenated Silicon | 49,736 |
| Thermal Energy Storage Using Perlite Saturated with a Phase Change Material | 45,589 |
| A New, Off-Peak Electric Storage Appliance for Commercial and Residential Use | 49,742 |
| A Computer Model for Processing of Thermoplastic Composites | 49,160 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| Materials Properties, Behavior, Characterization or Testing (continued) | |
| Phase II Projects: (First Year) | |
| A Position Sensitive Neutron Detector Using Boron Phosphide Semiconductor Sensors | 500,000 |
| Photoconductive Semiconductor Switch Flashover Suppression | 499,864 |
| The Effect of Polymer Additives and Residual Elements on the Cryogenic Performance and Radiation Resistance of Insulators for High-Field Magnets | 500,000 |
| Application of Neural Networks for Automated Inspection of Nuclear Power Plant Piping | 486,896 |
| Electrochemical Natural Gas Conversion to More Valuable Species | 499,997 |
| Novel Membranes for Natural Gas Liquids Recovery | 500,000 |
| Low Cost and Improved Carbon Composites for Phosphoric Acid Fuel Cells | 498,415 |
| Characterization of Phase I Preform/Composites in Ceramic Matrices Inserted by Chemical Vapor Infiltration and Other Alternative Infiltrating Processes | 499,330 |
| Phase II Projects: (Second Year) | |
| (none) | |
| Device or Component Fabrication, Behavior, or Testing | $4,997,478 |
| Phase I Projects: | |
| A Ceramic Filter for Removal of Particulates from Flue Gas | 49,844 |
| A Ceramic Filter for Removal of Particulates from Hot Gas Streams | 49,844 |
| A Facilitated Transport Membrane for Hot Coal Gas Desulfurization | 50,000 |
| Development of a Flue Gas Desulfurization Process Using a Novel Regenerative Hydrogen Bromide System | 49,999 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| Device or Component Fabrication, Behavior, or Testing (continued) | |
| Phase I Projects: (continued) | |
| Perovskite Solid Electrolytes for Intermediate Temperature Fuel Cells | 49,785 |
| An Advanced Design and Technique for a Low Cost, High Performance, Planar Solid Oxide Fuel Cell | 50,000 |
| Dehydration of Natural Gas by a Membrane Process | 49,993 |
| An Ultrafast Scintillator for Well Logging Applications | 46,012 |
| Development of Flexible Super-Lattice Artificial Crystals for Use in Fixed-Source Johann X-Ray Spectrometers with Application to Analytical Transmission Electron Microscopy | 49,984 |
| An Efficient X-Ray Wavelength Spectrometer for Improved Elemental Analysis on the Analytical Electron Microscope | 49,855 |
| Holographic Nano-Lithography of Semiconductors with the X-Ray Laser | 49,999 |
| Saddle Toroid Array Homogenizing Mirrors for Synchrotron Based X-Ray Lithography | 49,500 |
| Time and Position Sensitive Detectors for Instrumentation | 49,108 |
| Multilayer Coated X-Ray Diffraction Structures | 49,581 |
| Development of a Reliable and Safe Cryogenic Coupling with Automatic Check Valves and Insulating Overlap | 50,000 |
| An Application Specific, Discrete Junction Field Effect Transistor for Use in Large Particle Detector Preamplifier Circuitry | 50,000 |
| A Multi-Wavelength Holo-Fiber Optical Bus | 49,944 |
| A Fiber Optic Long Counter | 45,184 |
| Advanced High-Concentration High-Efficiency Tandem Photovoltaic Assemblies | 49,902 |
| Advanced Electrical Safety Components for Alternative Energy Power Systems | 48,500 |
| A Rugged Fiber Optic Connector Array for Severe Nuclear Plant Environments | 49,955 |

## OFFICE OF ENERGY RESEARCH (Continued)

| | FY 1990 |
|---|---|
| Device or Component Fabrication, Behavior, or Testing (continued) | |
| Phase II Projects: (First Year) | |
| A Low Damage SiC Grating for Synchrotron Radiation by Photoelectrochemical Etching | 500,000 |
| A Fast Direct Encoding Position-Sensitive Detector | 499,148 |
| A Superconducting Magnet for a Quasi-Optical Gyrotron | 500,000 |
| Phase II Projects: (Second Year) | |
| Large Area Hydrogenated Amorphous Silicon Thin Film Particle Detectors | 500,000 |
| Ultra High Resistivity Silicon Crystals for Radiation Detectors | 467,558 |
| A Laser Surface Profilometer for Steep Aspheric Surfaces | 496,452 |
| A Non-Contacting Dimensional Profiler | 497,331 |
| The Development of a Method for Greatly Increasing the Count-Rate Capability and Endurance of Position-Sensitive Detector Systems | 500,000 |

## OFFICE OF ENERGY RESEARCH

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

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

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

- Office of Basic Energy Sciences: Division of Engineering and Geosciences; Division of Materials Sciences; Division of Advanced Energy Projects
- Office of Health and Environmental Research: Division of Physical and Technologies Research
- Office of Fusion Energy
- Small Business Innovation Research Program

## Office of Basic Energy Sciences

### Division of Materials Sciences

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

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

There are three subprograms:

- Metallurgy and Ceramics seeks to understand the synergistic relationship between properties/behavior, structure, and processing parameters of materials.
- Solid State Physics is concerned with understanding the interactions of electrons, atoms, and defects and their role in determining the structure and properties of condensed matter.
- Materials Chemistry focuses on understanding the chemical properties of materials and their relationship to composition, structure, and specimen environment.

The operating funds for FY 1990 for the Division of Materials Sciences were $198,400,000. This was allocated to 434 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1990 was:

| | $ (Millions) |
|---|---|
| Materials Preparation, Synthesis, Deposition, Growth or Forming | 21.5 |
| Materials Structure and Composition | 28.6 |
| Materials Properties, Behavior, Characterization or Testing | 84.1 |
| Device or Component Fabrication, Behavior or Testing | -- |
| Facilities | 64.2 |

Division of Engineering and Geosciences

Materials research in the Division of Engineering and Geosciences is sponsored by two different research programs, as described below.

The BES Engineering Research Program was started in 1979 to help resolve the numerous serious engineering issues arising from efforts to meet U.S. energy needs. The program supports fundamental research on broad, generic topics in energy related engineering topics not as narrowly scoped as those addressed by the shorter term engineering research projects sponsored by the various DOE technology programs. Special emphasis is placed on projects which, if successfully concluded, will benefit more than one energy technology.

The broad goals of the BES Engineering Research Program are: (1) To extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and (2) To broaden the technical and conceptual base for solving future engineering problems in the energy technologies. The DOE contact for this Program is Oscar P. Manley, (301) 353-5822.

The BES Geosciences Research Program supports research that is fundamental in nature and of long-term relevance to one or more energy technologies, national security, energy conservation, or the safety objectives of the Department of Energy. It is also concerned with the extraction and utilization of such resources in an environmentally acceptable way. The purpose of this program is to develop geoscience or geosciences-related information relevant to one or more of these Department of Energy objectives or to develop the broad, basic understanding of geoscientific materials and processes necessary for the attainment of long-term Department of Energy goals. In general, individual research efforts supported by this program may involve elements of several different energy objectives. The DOE contact for this Program is William C. Luth, (301) 353-5822.

Materials Properties, Behavior, Characterization or Testing

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

- Demonstrate a composite multiviewing NDE transducer.
- Approach uses recent advances in ultrasonic scattering and inversion theories.
- Reconstruction protocol fits acquired data to an "equivalent" ellipsoid (3 axes and 3 angles).

194. 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.

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

- Phenomenological description of the nucleation and growth of microdefects in a metallic solid and their influence on the mechanical response.
- Investigation of the interaction of fiscuous effects (reflecting boundary slip) and the brittle effects (growth of microcracks). Problems in creep rupture and fatigue will be considered using the continuum damage model developed.

196. Transport in Porous/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.

197. Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding - DOE Contact Oscar P. Manley, (301) 353-5822; University of Connecticut Contact E. H. Jordan, (203) 486-2371

- Development and verification of a model of the time and history dependent viscoplastic deformation behavior of polycrystalline metals.
- Use data from high temperature experiments on polycrystalline Hastelloy-X to verify the model.
- Illuminate the role of grain boundary sliding in the overall deformation during complex load histories.

198. A Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding - DOE Contact Oscar P. Manley, (301) 353-5822; Engineering Science Software, Inc., Contact K. P. Walker, (401) 231-3182

- Develop a viscoplastic constitutive model, with accompanying FORTRAN software, to model the deformation behavior of polycrystalline metals comprised of an aggregate of face centered cubic single crystal grains whose crystallographic axes are oriented at random.

199. 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.

200. Plasma-Particle Interactions - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts C. B. Shaw, (208) 526-8818, S. C. Snyder, (208) 526-1507 and L. D. Reynolds, (208) 526-8335

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

201. Modeling of Thermal Plasma Processes - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts J. D. Ramshaw, (208) 526-9240 and C. H. Chang, (208) 526-2886

- Develop a comprehensive computational model of thermal plasma processes and plasma-particle interactions to provide an understanding of the space- and time-resolved flow and temperature distributions in the plasma plume and of the interaction between the plasma and particulate phase.
- Optimization of thermal plasma processing techniques.

202. Nondestructive Evaluation of Superconductors - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contact K. L. Telschow, (208) 526-1264

- Perform fundamental research leading to the development and application of new nondestructive evaluation (NDE) techniques and devices for the characterization of high temperature superconductors.
- Emphasis is on correlation of AC induced and DC transport current measurement data with material microstructure information and other measurements, using London and "Critical State" models of supercurrent flow.

203. Intelligent Control of Thermal Processes - DOE Contact Oscar P. Manley, (301) 353-5822; Idaho National Engineering Laboratory Contacts H. B. Smartt, (208) 256-8333 and J. A. Johnson, (208) 526-9021

- Develop model of gas metal arc welding process suitable for real-time process control
- Develop optical sensing capability to provide weld-bead geometry data.

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

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

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

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

205. Heat Transfer to Aqueous Polymer Solutions - DOE Contact Oscar P. Manley, (301) 353-5822; University of Illinois at Chicago Contact J. P. Hartnett, (312) 966-4490

- Investigate the fluid mechanical and heat transfer behavior of viscoelastic aqueous polymer solutions in order to predict the behavior of such fluids.

206. Pulse Propagation in Inhomogeneous Optical Fibers - DOE Contact Oscar P. Manley, (301) 353-5822; University of Maryland Contact C. Menyuk, (301) 455-3501

- Study the effects of slowly varying inhomogeneities and localized imperfections in optical fibers on their transmission properties.

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

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

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

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

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

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

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

- Develop sensing and control methods for gas-metal arc welding processes

- Model forces controlling metal transfer.

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

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

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

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

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

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

214. Low Resistivity Ohmic Contacts Between Semiconductors and High-Tc Superconductors - DOE Contact Oscar P. Manley, (301) 353-5822; National Institute of Standards and Technology Contacts J. Moreland, (303) 497-3641 and J. W. Ekin, (303) 497-5448

- Fabricate and characterize high-Tc superconductors/semiconductor contacts.
- Develop a method for optimizing the current capacity of such contacts to extend the application of high-Tc superconductors to hybrid superconductor-semiconductor technologies.

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

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

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

- Application of the scattered field approach to the detection of a cracklike flaw, and to the determination of its location, size, shape and orientation. Interior, as well as surface-breaking and near-surface cracks, are considered.
- Mathematical modeling of ultrasonic wave scattering by cracks adjusted to account for several typical characteristics of fatigue and stress-corrosion cracks, and the environment of such cracks.
- Investigation of local anisotropy and inhomogeneity due to near-tip voids and the effect of a zone of plastic deformation near a crack tip.

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

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

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

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

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

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

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

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

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

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

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

- Diagnose nonequilibrium reactive plasma.

- Application of PACVD processes to hard face coatings.

223. Thermodynamics of High Temperature Brines - DOE Contact William C. Luth, (301) 353-5822; Lawrence Berkeley Laboratory Contact K. S. Pitzer, (415) 642-3472

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

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

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

224. Studies of the Interactions Between Mineral Surfaces and Ions in Solution - DOE Contact William C. Luth, (301) 353-5822; Lawrence Berkeley Laboratory Contact D. L. Perry, (415) 486-4819

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

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

225. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions - DOE Contact William C. Luth, (301) 353-5822; Lawrence Livermore National Laboratory Contact D. G. Miller, (415) 422-8074

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

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

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

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

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

227. Solubilities of Calcite and Dolomite in Hydrothermal Solutions - DOE Contact William C. Luth, (301) 353-5822; Oak Ridge National Laboratory Contact D. R. Cole, (615) 574-5473

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

228. Salinity Effects on Oxygen and Hydrogen Isotope Partitioning Between Geothermal Brines and Other Phases at Elevated Temperatures - DOE Contact William C. Luth, (301) 353-5822; Oak Ridge National Laboratory Contact D. J. Wesolowski, (615) 574-6903

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

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

229. Advective-Diffusive/Dispersive Transport of Chemically Reacting Species in Hydrothermal Systems - DOE Contact William C. Luth, (301) 353-5822; University of California, Berkeley Contact H. C. Helgeson, (415) 642-1251

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

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

230. Rock Mechanics: Thermal Stress Microfracturing of Crystalline and Sedimentary Rocks - DOE Contact William C. Luth, (301) 353-5822; LLNL Contact B. P. Bonner, (415) 422-7080

- Acoustic emissions in brittle materials.

- Frequency dependent ultrasonic velocity.

231. Diffusion in Silicate Materials - DOE Contact William C. Luth, (301) 353-5822; LLNL Contact F. J. Ryerson, (415) 422-6170

- Diffusion profiles in silicate minerals at 600C<T<900C.
- Using ion implantation.
- Radiation damage increased diffusion coefficients.
- Activation energies comparable to published data.

232. Rheology of Melts - DOE Contact William C. Luth, (301) 353-5822; University of California at Santa Barbara Contact F. J. Spera, (805) 893-8649; University of Minnesota Contact D. A. Yuen, (612) 624-1868

- Rheology of silicate melts and crystal-liquid mixtures.
- Presence/absence of dilute concentrations of gas bubbles.
- Directed toward understanding caldera-type volcanic eruptions.
- Involves modeling using a large-amplitude Lagrangian formulation.

233. Microcrack Growth in Crystalline Rock - DOE Contact William C. Luth, (301) 353-5822; Lawrence Berkeley Laboratory Contact L. R. Myer, (415) 486-6456

- Mechanism of microcrack growth in brittle rocks.
- Compressive triaxial stress.
- Role of pore collapse and compaction.

234. Experimental Database and Predictive Theories for Thermodynamic Properties of Aqueous Solutions - DOE Contact William C. Luth, (301) 353-5822; University of Delaware Contact R. H. Wood, (302) 451-2941

- Measurements of apparent molar heat capacity of aqueous solutions of $H_2S$, $CO_2$ and $CH_4$ at twelve temperatures from 25 to 450°C and at pressure near 350 bar.

- Measurement of apparent molar volume of same solutions at same temperatures and two different pressures.

- Investigation of theoretical models capable of representing these data and extrapolating them to higher temperatures and pressures.

235. Physical Characterization of Magma Samples - DOE Contact William C. Luth, (301) 353-5822; University of Hawaii at Manoa Contact M. H. Manghnani, (808) 948-7825

- Application of ultrasonic interferometry to measure velocity and attenuation in natural and synthetic silicate melts.

- Investigation of interrelationships between physical, elastic and anelastic, and thermodynamic properties of silicate melts.

- Development of a Brillouin scattering technique for measuring the elastic and anelastic properties of melts.

236. Investigations of Ultrasonic Surface Wave Interaction with Porous Saturated Rocks - DOE Contact William C. Luth, (301) 353-5822; Ohio State University Contact L. Adler, (614) 292-1974

- Investigation of the interaction of ultrasonic waves with fluid-saturated porous solids.

- Numerical calculations of energy transmission and reflection coefficients for interface formed by two porous media with different porosities. Demonstration that the reflected or transmitted slow wave is strongly affected by pore interface conditions.

- Theoretical and experimental investigation of leaky Lamb wave interaction with a fluid-saturated porous plate.

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

- Study of the relationship between hydrothermally induced mobility of uranium and lead isotopes and the chemical and mechanical properties of small populations of zircons ($ZrSiO_4$).
- Demonstrated removal of 30-40 percent of uranium from the zircon by treatment with 2M NaCl, as compared with less than 10 percent by treatment with 2 percent $HNO_3$.

238. PVTX Properties of Fluid Systems: $NaCl\text{-}CaCl_2\text{-}H_2O$ - DOE Contact William C. Luth, (301) 353-5822; Virginia Polytechnic Institute and State University Contact R. J. Bodnar, (703) 961-7455

- Goal is to accurately and completely determine the PVTX properties of geologically important fluid systems over the complete range of conditions relevant to the Earth's crust.
- Completed studies of $NaCl\text{-}H_2O$ and $NaCl\text{-}KCl\text{-}H_2O$. Near completion for $NaCl\text{-}H_2O\text{-}CO_2$. Planned studies of phase equilibria and volumetric properties of $NaCl\text{-}CaCl_2\text{-}H_2O$.

Materials Structure and Composition

239. Silicate Thermochemistry - DOE Contact William C. Luth, (301) 353-5822; Princeton University Contact A. Navrotsky, (609) 452-4674

- Examination of the effects of the charge coupled substitution $Si^{4+} = T^{3+}Na^{1+}$ (T = Al, B, Fe and Ga) on the overall stabilization of framework silicate glasses in the systems $xNaTO_2\text{-}(1\text{-}x)SiO_2$.
- Development of a technique for solution calorimetry of oxides of highly charged cations in molten $2PbO \cdot B_2O_3$. Measurement of thermodynamic mixing properties of glasses of the system $K_2O\text{-}SiO_2\text{-}La_2O_3$.
- Investigation of the structural and thermodynamic effects of aluminum substitution on tri-octahedral Fe-free micas.

Division of Advanced Energy Projects

Materials Preparation, Synthesis, Deposition, Growth or Forming

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

- Deposition of films by "seeding" atoms or molecules into a free jet expansion, e.g., of helium, and directing the jet at a substrate at relatively high pressure.

- Fundamentals of gas jet deposition being explored, in particular its high rate and impact energy control.

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

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

- Emphasize bismuth-containing compounds.

Materials Properties, Behavior, Characterization or Testing

242. Production of Fuels and Chemicals From Methane - DOE Contact Walter M. Polansky, (301) 353-5995; Argonne National Laboratory Contact Victor A. Maroni, (708) 972-4547

- Novel bifunctional catalyst materials are being developed that can convert methane into fuels and industrial chemicals under moderate conditions of temperature and pressure.

- The types of catalysts under investigation are molecular sieve materials that are incorporated with transition metals having unique oxidation state chemistries and coordination geometry.

Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program was established in compliance with the Small Business Innovation Development Act of 1982, Public Law 97-219. The program is designed for implementation in a three-phase process, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is about six months and awards are limited to $50,000. Phase II is the principal research or research and development effort, and awards can be as high as $500,000 for work to be performed in periods of up to two years. Under Phase III, commercial applications of the research or research and development are to be pursued by small businesses with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or processes desired by the Government.

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

The work supported in this program represents high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE SBIR projects (not just those of interest in materials research) are given in the following publications: Abstracts of Phase I Awards, 1990 (DOE/ER-0472), Abstracts of Phase II Awards, 1990 (DOE/ER-0467), and Abstracts of Phase II Awards, 1989 (DOE/ER-0418). 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:

Low Cost Iron Microparticles for Slurry Catalyzed Coal Liquefaction - DOE Contact William Peters, (412) 675-6597; ElectroChem, Inc. Contact Dr. Vinod Jalan, (617) 932-3383

Improved Enhanced Oil Recovery Processes Using Novel Synthetic Copolymers Containing Large Amounts of Acrylamide - DOE Contact Jerry Casteel, BPO, (918) 337-4412; R. L. Clampitt and Associates Contact M. L. Clampitt, (918) 333-3020

Single Crystal Molybdenum Mirrors for High Power Vacuum Ultraviolet and X-Ray Radiation - DOE Contact Jerry Smith, (301) 353-4269; INRAD, Inc. Contact Dr. Warren Ruderman, (201) 767-1910

Ultrafine Grained Molybdenum Silicide with Ultrafine Hafnium Carbide Dispersoids for Improved Superplastic Formability - DOE Contact Jerry Smith, (301) 353-4269; Marko Materials, Inc. Contact Dr. Ranjan Ray, (508) 663-2210

A Large Area, Position Sensitive Detector for Synchrotron X-Ray Diffraction - DOE Contact Jerry Smith, (301) 353-4269; Radiation Monitoring Devices, Inc. Contact Dr. Michael R. Squillante, (617) 926-1167

Gas Jet Injection of Clusters into Liquids - DOE Contact Jerry Smith, (301) 353-4269; Schmitt Technology Associates Contact Dr. Bret L. Halpern, (203) 786-5130

Silicon Carbide Coatings for Synchrotron Optics - DOE Contact Jerry Smith, (301) 353-4269; Spire Corporation Contact Lawrence Stelmack, (617) 275-6000

Innovative Mirror Technology for X-Ray Reflective Optics - DOE Contact Jerry Smith, (301) 353-4269; Superior Vacuum Technology Contact Dr. Peter Chow, (612) 941-1929

A Method of Producing Carbon Clusters - DOE Contact Jerry Smith, (301) 353-4269; TDA Research, Inc. Contact Dr. J. Thomas McKinnon, (303) 422-1338

Strength, Reliability, and Surface Hardness Improvement of Structural Ceramics Through Ion Implantations - DOE Contact Jerry Smith, (301) 353-4269; Universal Energy Systems, Inc. Contact Dr. Rabi S. Bhattacharya, (513) 426-6900

Thin Film Tungsten Diselenide Photoelectrodes - DOE Contact Robert Marianelli, (301) 353-5804; Advanced Technology Materials, Inc. Contact Dr. Walter P. Kosar, (203) 355-2681

Development of High-Performance Chemically Resistant Composite Membranes - DOE Contact Robert Marianelli, (301) 353-5804; Bend Research, Inc. Contact Dr. Scott B. McCray, (503) 382-4100

Molecular Recognition in Metal Ion Sensors - DOE Contact Robert Marianelli, (301) 353-5804; Marko Materials, Inc. Contact Dr. Ranjan Ray, (508) 663-2210

Ultrathin Metal Membranes - DOE Contact Robert Marianelli, (301) 353-5804; Membrane Technology and Research, Inc. Contact Dr. Amulya Athayde, (415) 328-3338

Development of Oxidation-Resistant Mosaic Membranes with Enhanced Transport Properties - DOE Contact Robert Marianelli, (301) 353-5804; Separation Systems Technology, Inc. Contact Robert L. Riley, (619) 581-3765

A Diamond X-Ray Detector - DOE Contact Charles Finfgeld, (301) 353-3421; Advanced Technology Materials, Inc. Contact Dr. Charles P. Beetz, Jr., (203) 355-2681

Changes in Niobium Tin Conductors Made by the Internal Tin Method to Improve Magnet Performance - DOE Contact T. V. George, (301) 353-4957; IGC Advanced Superconductors, Inc. Contact Gennardy M. Ozyeransky, (203) 753-5215

Alternative Fabrication Processes for Ultrafine Filament, Metal Matrix Microcomposites - DOE Contact T. V. George, (301) 353-4957; Supercon, Inc. Contact Charles Renaud, (508) 842-0174

A Novel Carbon First Wall Material - DOE Contact Robert Price, (301) 353-3565; Applied Sciences, Inc. Contact Max L. Lake, (513) 767-1477

Development of Radiation-Resistant Copper Matrix Composites - DOE Contact Robert Price, (301) 353-3565; Materials and Electrochemical Research Corporation Contact Dr. J. C. Withers, (602) 574-1980

Initial Exploration of Amorphous and Polycrystalline Silicon Thin Film Transistors as Preamplifiers for Particle Detector Applications - DOE Contact Jay Benesch, (301) 353-4993; Glasstech Solar, Inc. Contact Dr. Dashen Shen, (303) 425-6600

Development of New Radiation Resistant Fluors with Large Stokes Shift and High Quantum Efficiency - DOE Contact Jay Benesch, (301) 353-4993; Nanoptics, Inc. Contact Dr. J. Harmon, (904) 392-7105

Low Cost, Large Area Epitaxial Silicon Detectors for Sampling Calorimeters - DOE Contact Jay Benesch, (301) 353-4993; Spire Corporation Contact Orlando DeSilvestre, (617) 275-6000

Economic Low Loss Niobium Tin for Pulsed Field Applications, Made by a Modified Internal Tin Process - DOE Contact Gerald Peters, (301) 353-5228; IGC Advanced Superconductors; Inc. Contact Dr. Eric Gregory, (203) 574-7988

Development of Practical Multifilamentary Superconductors Using Chevrel Phase Materials for Magnet Applications at More Than 20 Tessla - DOE Contact Gerald Peters, (301) 353-5228; Supercon, Inc. Contact Dr. James Wong, (508) 842-0174

A Thallium-Barium-Calcium-Copper Oxide, Thin Film, Superconducting Radio Frequency Cavity - DOE Contact Stanley Whetstone, (301) 353-3613; Advanced Technology Materials, Inc. Contact Dr. Peter S. Kirlin, (203) 355-2681

Superconducting Radio Frequency Cavity Coatings by Metallorganic Chemical Vapor Deposition - DOE Contact Stanley Whetstone, (301) 353-3613; Spire Corporation Contact Dr. Anton C. Greenwald, (617) 275-6000

New Scintillator Materials - DOE Contact Stanley Whetstone, (301) 353-3613; ALEM Associates Contact Dr. A. Lempicki, (617) 236-1025

Scintillating Optical Fibers of Barium Fluoride for Nuclear Instrumentation - DOE Contact Stanley Whetstone, (301) 353-3613; LaserGenics Corporation Contact Dr. Richard G. Schlecht, (408) 433-0161

A New Semiconductor Photosensor for Scintillation Spectroscopy - DOE Contact Stanley Whetstone, (301) 353-3613; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Highly Parallel, High Bandwidth, Optical Holographic Analog-to-Digital Convertors - DOE Contact Richard Rinkenberger, (301) 353-3613; Physical Optics Corporation Contact Dr. Freddie Lin, (213) 320-3088

Electrodeposition of Silicon Films from Liquid-Metal Solutions for Photovoltaic Applications - DOE Contact Alec Bulawka, (202) 586-5633; AstroPower, Inc. Contact Dr. Michael G. Mauk, (302) 366-0400

Magnetically Enhanced Plasma Deposition of Intrinsic Hydrogenated Amorphous Silicon Layers in Roll-to-Roll Systems - DOE Contact Alec Bulawka, (202) 586-5633; Iowa Thin Film Technologies, Inc. Contact Dr. Frank R. Jeffrey, (515) 294-7732

Thermally Conductive, Solid-State Thermal Energy Storage Materials With High Latent Heats - DOE Contact Sam Tagore, (202) 586-9210; Cape Cod Research, Inc. Contact Dr. Brian G. Dixon, (508) 759-5911

Innovative Methods for the Production of Polymers from Biobased Materials - DOE Contact Stanley Wolf, (202) 586-1514; Advanced Fuel Research, Inc. Contact Dr. Michael A. Serio, (203) 528-9806

Development of a Low Cost, Continuous, Elastic, Reservoir Process to Produce Composite Sandwich Panels - DOE Contact Stanley Wolf, (202) 586-9806; Foster-Miller, Inc. Contact Jack Woods, (617) 890-3200

A Novel Precursor Yarn for Advanced Automotive Composite Structures - DOE Contact Stanley Wolf, (202) 586-9806; Pepin Associates, Inc. Contact John N. Pepin, (207) 883-8338

Structural Tannin-Based Lumber End-Joint Adhesives for Existing Product Lines - DOE Contact Stanley Wolf, (202) 586-9806; Roland E. Kreibich Consulting Service Contact Dr. Roland E. Kreibich, (206) 838-0964

Polypropylene Composites Reinforced with Biobased Graft Polymer - DOE Contact Stanley Wolf, (202) 586-9806; Southeastern Reduction Company Contact John D. Nizio, (912) 244-1324

Property-Enhanced Composites from Lignocellulosic Fibers - DOE Contact Stanley Wolf, (202) 586-9806; Xylan, Inc. Contact Laura L. Jelle, (608) 238-4600

Fiber Optic Bus-Organized Systems for Sensor Data Acquisition and Validation - DOE Contact John Lewellen, (301) 353-3684; American Micro-Optical, Inc. Contact Dr. Marcos Kleinerman, (508) 765-1228

Phase II Projects: (First Year)

Low Temperature Processing of High $T_c$ Superconductor Films for Integration of Detector Arrays with Silicon Circuitry - DOE Contact Walter Polansky, (301) 353-5995; Advanced Fuel Research, Inc. Contact Dr. David G. Hamblen, (203) 528-9806

Improved Thin Film Multilayer Coatings for Thermal Neutron Guides - DOE Contact Jerry Smith, (301) 353-4269; Opto-Line Associates, Inc. Contact John H. Bradshaw, (508) 470-3275

Development of a Fabrication Process which Demonstrates the Commercial Feasibility of Supermirror Coatings for Neutron Guides - DOE Contact Jerry Smith, (301) 353-4269; Ovonic Synthetic Materials Company Contact James L. Wood, (313) 326-1290

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

Development of Internal Tin $Nb_3Sn$ Conductors by Novel Manufacturing Techniques - DOE Contact Earle Fowler, (301) 353-4801; IGC Advanced Superconductors, Inc. Contact Dr. Eric Gregory, (203) 574-7988

Ultrafine Filament NbTi Superconductors - DOE Contact Jay F. Benesch, (301) 353-4993; IGC Advanced Superconductors, Inc. Contact Dr. Hem Kanithi, (203) 753-5215

A Radiation Resistant Cryogenic Temperature Sensor for the 4K to 80K Range - DOE Contact Jay Benesch, (301) 353-4993; Lake Shore Cryotronics, Inc. Contact Dr. Philip R. Swinehart, (614) 891-2243

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

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

Recyclable Molds for Casting Nuclear Fuel - DOE Contact Clinton Bastin, (301) 353-4259; Advanced Technology Materials, Inc. Contact Dr. Ward C. Stevens, (203) 355-2681

Ceramic Composite Materials for Pyrometallurgical Reprocessing - DOE Contact Clinton Bastin, (301) 353-4259; Materials and Electrochemical Research Corporation Contact Dr. R. O. Loutfy, (602) 574-1980

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

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

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

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

Polymer Solid Electrolytes with Specific Cation Conduction - DOE Contact Albert Landgrebe, (202) 586-1483; Moltech Corporation Contact Dr. Terje A. Skotheim, (516) 282-4490

Phase II Projects: (Second Year)

A Mass Production Facility for Plastic Scintillating Optical Fibers with Radiation-Hardened Properties for the Superconducting Super Collider - DOE Contact Jay Benesch, (301) 353-4993; Bicron Corporation Contact Charles R. Hurlbut, (216) 564-2251

A Ceramic Membrane for Gas Separations - DOE Contact Dan Cicero, METC, (304) 291-4826; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

Radiation-Modified Pyroelectric Conversion Materials - DOE Contact Richard Kelley, (301) 353-3426; Chronos Research Laboratories, Inc. Contact Dr. Randall B. Olsen, (619) 455-8200

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

Materials Properties, Behavior, Characterization or Testing

Phase I Projects:

Development of Computer-Controlled Scanning Electron Microscopy Techniques for Predicting the Cleaning Behavior of Coal - DOE Contact Gino Irdi, PETC, (412) 892-5956; R. J. Lee Group, Inc. Contact Gary S. Casuccio, (412) 325-1776

Utilization of Fluidized Bed Residuals for Producing Synthetic Aggregate by Vacuum Extrusion - DOE Contact Jerry L. Harness, METC, (304) 291-4835; Valley Forge Laboratories, Inc. Contact Robert J. Collins, (215) 688-8517

An Evaluation in a Simulated Fluidized-Bed Combustion Environment of Erosion Resistance of Coatings Applied Using a Hypersonic Spray Process - DOE Contact Gary A. Nelken, METC, (304) 291-4216; Holtgren, Inc. Contact Dr. Edward R. Buchanan, (201) 686-2332

A Holographic and Reflection X-Ray Laser Microscope for Lithographic Inspection - DOE Contact Walter Polansky, (301) 353-5995; Princeton X-Ray Laser, Inc. Contact Dr. R. J. Rosser, (201) 329-0505

Subsurface Gamma Ray Backscatter Scanning Microscopy - DOE Contact Jerry Smith, (301) 353-4269; Spire Corporation Contact Dr. Charles Blatchley, (617) 275-6000

Three-Dimensional Inspection of First Wall Surfaces for the Compact Ignition Tokamak - DOE Contact Robert Price, (301) 353-3565; Intelligent Automation Systems, Inc. Contact Dr. Steven J. Gordon, (617) 354-3830

A Technique for Measuring Diffusion of Hydrogen Isotopes in Oxides - DOE Contact Robert Price, (301) 353-3565; Ionwerks Contact J. Albert Schultz, (713) 522-9880

Failure Criteria for Drawing and Extrusion of Trimetal Superconducting Composite Wire - DOE Contact Jay Benesch, (301) 353-4993; Metalforming, Inc. Contact Dr. Betzalel Avitzur, (215) 391-1338

Piezoelectrically Driven Micropositioners for Rotation at Normal and Cryogenic Temperature in High Magnetic Fields - DOE Contact Jay Benesch, (301) 353-4993; Micro Pulse Systems, Inc. Contact Charles W. Staufenberg, Jr. (805) 687-6558

Nondestructive Evaluation of Superconducting Magnet Wire Using a Scanning Acoustic Pulse Spectroscope - DOE Contact Jay Benesch, (301) 353-4993; Sonoscan, Inc. Contact Dr. Albert C. Wey, (708) 766-7088

A Novel, Robust, High Repetition, High Brightness Cathode - DOE Contact Gerald Peters, (301) 353-5228; Integrated Applied Physics, Inc. Contact George Kirkman, (818) 821-0652

An All-Solid-State Titanium-Doped Sapphire Laser Source for Production of Polarized Electrons - DOE Contact Gerald Peters, (301) 353-5228; Lightwave Electronics Corporation Contact Dr. Thomas R. Steele, (415) 962-0755

In-Situ Diagnostic Technique for Process Monitoring and Control of the Plasma Deposition of Amorphous Hydrogenated Silicon - DOE Contact Alec Bulawka, (202) 586-5633; Advanced Fuel Research, Inc. Contact Dr. Philip W. Morrison, Jr., (203) 528-9806

Thermal Energy Storage Using Perlite Saturated with a Phase Change Material - DOE Contact Sam Tagore, (202) 586-9210; Energy Science Laboratories, Inc. Contact Eric R. Pulliam, (619) 455-4688

A New, Off-Peak Electric Storage Appliance for Commercial and Residential Use - DOE Contact Sam Tagore, (202) 586-9210; Thermal Electric Devices, Inc. Contact Dr. Edward Redding, (505) 345-3636

A Computer Model for Processing of Thermoplastic Composites - DOE Contact Stanley Wolf, (202) 586-1514; Applied Polymer and Biotechnology Consultants Contact Dr. J. Naghizadeh, (415) 592-1321

Phase II Projects: (First Year)

A Position Sensitive Neutron Detector Using Boron Phosphide Semiconductor Sensors - DOE Contact Jerry Smith, (301) 353-4269; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Photoconductive Semiconductor Switch Flashover Suppression - DOE Contact David Sutter, (301) 353-5228; Tetra Corporation Contact Dr. Juan M. Elizondo, (505) 345-8623

The Effect of Polymer Additives and Residual Elements on the Cryogenic Performance and Radiation Resistance of Insulators for High-Field Magnets - DOE Contact T. V. George, (301) 353-4957; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 447-2226

Application of Neural Networks for Automated Inspection of Nuclear Power Plant Piping - DOE Contact John Lewellen, (301) 353-3684; Karta Technology, Inc. Contact Dr. G. P. Singh, (512) 681-9102

Electrochemical Natural Gas Conversion to More Valuable Species - DOE Contact Harold Shoemaker, (304) 291-4715; Eltron Research, Inc. Contact Dr. Anthony F. Sammells, (708) 898-1583

Novel Membranes for Natural Gas Liquids Recovery - DOE Contact Harold Shoemaker, METC, (304) 291-4715; Membrane Technology and Research, Inc. Contact Dr. Johannes G. Wijmans, (415) 328-2228

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

Characterization of Phase I Preform/Composites in Ceramic Matrices Inserted by Chemical Vapor Infiltration and Other Alternative Infiltrating Processes - DOE Contact James Carr, (301) 353-6519; Quadrax Advanced Materials Systems, Inc. Contact Dr. Robert A. Florentine, (401) 683-6600

Phase II Projects: (Second Year)

(none)

Device or Component Fabrication, Behavior, or Testing

Phase I Projects:

A Ceramic Filter for Removal of Particulates from Flue Gas - DOE Contact Thomas D. Brown, (412) 892-4691; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

A Ceramic Filter for Removal of Particulates from Hot Gas Streams - DOE Contact Curtis V. Nakaiski, (304) 291-4275; CeraMem Corporation Contact Dr. Robert L. Goldsmith, (617) 899-0467

A Facilitated Transport Membrane for Hot Coal Gas Desulfurization - DOE Contact Suresh C. Jain, (304) 291-4446; ElectroChem, Inc. Contact Dr. Vinod Jalan, (617) 932-3383

Development of a Flue Gas Desulfurization Process Using a Novel Regenerative Hydrogen Bromide System - DOE Contact Felixa Eskey, (412) 892-4769; Giner, Inc. Contact Dr. John A. Kosek, (167) 899-7270

Perovskite Solid Electrolytes for Intermediate Temperature Fuel Cells - DOE Contact William Huber, METC, (304) 291-4663; Eltron Research, Inc. Contact Dr. Anthony F. Sammells, (708) 898-1583

An Advanced Design and Technique for a Low Cost, High Performance, Planar Solid Oxide Fuel Cell - DOE Contact William Huber, METC, (304) 291-4663; Ztek Corporation Contact Dr. Michael Hsu, (617) 890-5665

Dehydration of Natural Gas by a Membrane Process - DOE Contact Harold Shoemaker, (304) 291-4715; Membrane Technology and Research, Inc. Contact Dr. J. G. Wijmans, (415) 328-2228

An Ultrafast Scintillator for Well Logging Applications - DOE Contact Harold Shoemaker, (304) 291-4715; TPL, Inc. Contact Dr. Larry A. Harrah, (505) 296-3648

Development of Flexible Super-Lattice Artificial Crystals for Use in Fixed-Source Johann X-Ray Spectrometers with Application to Analytical Transmission Electron Microscopy - DOE Contact Jerry Smith, (301) 353-4269; Multilayer Optics and X-Ray Technology, Inc. Contact Dr. Mark W. Lund, (801) 378-3972

An Efficient X-Ray Wavelength Spectrometer for Improved Elemental Analysis on the Analytical Electron Microscope - DOE Contact Jerry Smith, (301) 353-4269; Peak Instruments, Inc. Contact Dr. Nicholas C. Barbi, (609) 737-8133

Holographic Nano-Lithography of Semiconductors with the X-Ray Laser - DOE Contact Jerry Smith, (301) 353-4269; Princeton X-Ray Laser, Inc. Contact Dr. Joseph Blanc, (201) 329-0505

Saddle Toroid Array Homogenizing Mirrors for Synchrotron Based X-Ray Lithography - DOE Contact Jerry Smith, (301) 353-4269; Princeton X-Ray Laser, Inc. Contact Dr. Roy Rosser, (201) 329-0505

Time and Position Sensitive Detectors for Instrumentation - DOE Contact Jerry Smith, (301) 353-4269; Schmidt Instruments, Inc. Contact Dr. Howard K. Schmidt, (713) 529-9040

Multilayer Coated X-Ray Diffraction Structures - DOE Contact Jerry Smith, (301) 353-4269; X-Ray Instrumentation Associates Contact Dr. William K. Warburton, (415) 325-5779

Development of a Reliable and Safe Cryogenic Coupling with Automatic Check Valves and Insulating Overlap - DOE Contact Jay Benesch, (301) 353-4993; Meyer Tool and Manufacturing, Inc. Contact John Carusiello, (708) 425-9080

An Application Specific, Discrete Junction Field Effect Transistor for Use in Large Particle Detector Preamplifier Circuitry - DOE Contact Robert Woods, (301) 353-3367; InterFET Corporation Contact Larry A. Rehn, (214) 487-1287

A Multi-Wavelength Holo-Fiber Optical Bus - DOE Contact Robert Woods, (301) 353-3367; Physical Optics Corporation Contact Dr. Behzad Moslehi, (213) 320-3088

A Fiber Optic Long Counter - DOE Contact Stanley Whetstone, (301) 353-3613; Fibertek, Inc. Contact Dr. Garry Spector, (703) 471-7671

Advanced High-Concentration High-Efficiency Tandem Photovoltaic Assemblies - DOE Contact Alec Bulawka, (202) 586-5633; Kopin Corporation Contact Dr. Mark B. Spitzer, (508) 824-6696

Advanced Electrical Safety Components for Alternative Energy Power Systems - DOE Contact Alec Bulawka, (202) 586-5633; Silicon Energy Corporation Contact Richard T. West, (818) 700-1995

A Rugged Fiber Optic Connector Array for Severe Nuclear Plant Environments - DOE Contact John Lewellen, (301) 353-3684; Physical Optics Corporation Contact Dr. Behzad Moslehi, (213) 320-3088

Phase II Projects: (First Year)

A Low Damage SiC Grating for Synchrotron Radiation by Photoelectrochemical Etching - DOE Contact Jerry Smith, (301) 353-4269; EIC Laboratories, Inc. Contact Dr. Michael M. Carrabba, (617) 769-9450

A Fast Direct Encoding Position-Sensitive Detector - DOE Contact Stanley Whetstone, (301) 353-3613; Charles Evans and Associates Contact Dr. Bruce H. Newcome, (415) 369-4567

A Superconducting Magnet for a Quasi-Optical Gyrotron - DOE Contact T. V. George, (301) 353-4957; Intermagnetics General Corporation Contact W. Denis Markiewicz, (518) 457-5456

Phase II Projects: (Second Year)

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

Ultra High Resistivity Silicon Crystals for Radiation Detectors - DOE Contact Jay Benesch, (301) 353-4993; IntraSpec, Inc. Contact John Walter, (615) 483-1859

A Laser Surface Profilometer for Steep Aspheric Surfaces - DOE Contact Richard Kelley, (301) 353-3426; OPTRA, Inc. Contact Dr. Michael Hercher, (508) 921-2100

A Non-Contacting Dimensional Profiler - DOE Contact Stanley Sobczynski, (202) 586-1878; OPTRA, Inc. Contact Dr. Michael Hercher, (508) 921-2100

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

## OFFICE OF ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT

| | FY 1990 |
|---|---|
| Office of Environmental Restoration and Waste Management - Grand Total | $10,750,000 |
| Division of Waste Management Projects | $10,750,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $1,100,000 |
| Technical Support to West Valley Demonstration Project | $1,100,000 |
| Materials Properties, Behavior, Characterization or Testing | $9,650,000 |
| Materials Characterization Center Testing of West Valley Formulation Glass | 500,000 |
| Development of Test Methods and Testing of West Valley Reference Formulation Glass | 900,000 |
| Process and Product Quality Optimization for the West Valley Waste Form | 250,000 |
| Waste Form Qualification | 6,000,000 |
| Immobilization, Volume Reduction, and In-Place Stabilization | 2,000,000 |

## OFFICE OF ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT

In November 1989 the Department consolidated into a new Office of Environmental Restoration and Waste Management (EM) waste management and waste treatment activities formerly managed by portions of the Office of Nuclear Energy and the Office of Defense Programs. These activities include waste treatment technology and specific project operations.

### Division of Waste Management Projects

The objective of the Division of Waste Management Projects is to conduct waste management activities for ending interim storage of high-level waste and achieving permanent disposal of high-level waste. Defense wastes were generated by atomic energy defense activities at three Departmental operating locations: the Savannah River Site in South Carolina, the Hanford Site in Washington, and the Idaho National Engineering Laboratory in Idaho. Additionally, Congress directed the Department in 1980 to demonstrate the solidification of liquid high-level waste at West Valley (New York) which originated at the nation's only commercial plant to reprocess spent nuclear fuel. At all four sites there are major programs in various stages of completion which will immobilize the high-level waste preparatory to geologic disposal. All four projects are managed by this Division.

At Savannah River and West Valley, high-level waste will be immobilized in a borosilicate glass prepared in a liquid-fed ceramic joule-heated melter. Hanford is planning to use the same waste form and process, but the project is in the conceptual design stage. At Idaho, the merits of several alternative waste management strategies are being evaluated. A strategy will be selected in compliance with the National Environmental Policy Act (NEPA) process for disposal of Idaho high-level waste.

The Defense Waste Processing Facility at Savannah River is beginning nonradioactive operations in preparation for radioactive operation in 1993. West Valley is constructing the vitrification cell. For these two projects, materials research focuses on incremental improvements in the waste form durability based on a reference formulation chosen some time ago. Hanford project is now studying pre-treatment options for most effectively preparing the several chemically-varied types of waste for partition between a high-activity stream which will be vitrified and a low-activity stream which will be immobilized in a grout or cement waste form.

Materials Preparation, Synthesis, Deposition, Growth or Forming

243. Technical Support to West Valley Demonstration Project - DOE Contact T. W. McIntosh, (301) 353-7189; PNL Contact W. A. Ross, (509) 376-3644

- Characterizing operating conditions for ion exchange processes that remove cesium and plutonium from the high-level liquid supernate.

- Developing an empirical model which relates borosilicate glass composition to the chemical durability of the final waste form.

Materials Properties, Behavior, Characterization or Testing

244. Materials Characterization Center Testing of West Valley Formulation Glass - DOE Contact T. W. McIntosh, (301) 353-7189; PNL Contact S. G. Marschman, (509) 376-3569

- Evaluating chemical durability of glasses within the expected range of composition of the West Valley Demonstration Project borosilicate glass waste form.

245. Development of Test Methods and Testing of West Valley Reference Formulation Glass - DOE Contact W. S. Ketola, (716) 942-3414; CUA Contact P. B. Macedo, (202) 635-5326

- Developing test methods for nonradioactive and radioactive borosilicate glass waste forms.

- Maximizing the region of acceptable quality around the point of optimal durability for West Valley borosilicate glass waste form.

246. Process and Product Quality Optimization for the West Valley Waste Form - DOE Contact W. S. Ketola, (716) 942-4314; AU Contact L. D. Pye, (607) 871-2432

- Studying properties and crystallization behavior of West Valley borosilicate glass reference composition.

247. Waste Form Qualification - DOE Contact M. Dev, (509) 376-3412; WHC Contact S. Schaus, (509) 376-8365

- Providing fundamental data for start-up of Defense Waste Processing Facility and for acceptance of borosilicate glass waste form at a repository.

248. Immobilization, Volume Reduction, and In-Place Stabilization - DOE Contact M. Dev, (509) 376-3412; WHC Contact S. Schaus, (509) 376-8365

- Providing information about waste characterization, retrieval technology, and waste processing for high-level waste at Hanford and Idaho National Engineering Laboratory sites.

# OFFICE OF NUCLEAR ENERGY

| | FY 1990 |
|---|---|
| Office of Nuclear Energy - Grand Total | $128,634,000 |
| Office of Uranium Enrichment | $ 20,513,000 |
| Gaseous Diffusion | |
| Device or Component Fabrication, Behavior or Testing | $ 5,113,000 |
| Gaseous Diffusion: Barrier Quality | 2,053,000 |
| Gaseous Diffusion: Materials and Chemistry Support | 3,060,000 |
| Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS) | $ 15,400,000 |
| U-AVLIS: Separator Materials | 5,400,000 |
| U-AVLIS: Uranium Processing | 10,000,000 |
| Office of Civilian Reactor Development | $ 29,786,000 |
| Office of Advanced Reactor Programs | $ 3,430,000 |
| Division of High Temperature Gas-Cooled Reactors | $ 3,430,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 300,000 |
| Fuel Process Development | 300,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 3,130,000 |
| Fuel Materials Development | 260,000 |
| Fuel Development and Testing | 2,100,000 |
| Graphite Development | 50,000 |
| Graphite Development and Testing | 250,000 |

## OFFICE OF NUCLEAR ENERGY (Continued)

| | FY 1989 |
|---|---|
| Office of Advanced Reactor Programs (continued) | |
| Division of High Temperature Gas-Cooled Reactors (continued) | |
| Materials Properties, Behavior, Characterization or Testing (continued) | |
| Metals Technology Development | 30,000 |
| Structural Materials Development | 340,000 |
| Advanced Gas Reactor Materials Development | 100,000 |
| Office of Technology Support Programs (LMRs) | $26,356,000 |
| Fuels and Core Materials | $18,856,000 |
| Materials Properties, Behavior, Characterization or Testing | $18,856,000 |
| Fuel Performance Demonstration | 5,441,000 |
| Pyroprocess Development | 4,262,000 |
| Fuel Safety Experiments and Analysis | 3,187,000 |
| Core Design Studies | 947,000 |
| Fuel Cycle Studies | 3,674,000 |
| LMR Technology R&D | 1,345,000 |
| Structural Materials and Design Methodology | $ 7,500,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 7,500,000 |
| Structural Design/Life Assurance Technology (Funded by JAPC) | 0 |
| Modified 9 Cr-1 Mo Steel Design Properties (Funded by JAPC) | 0 |
| MOTA Fabrication and Operation | 1,200,000 |
| Absorber Development | 1,000,000 |
| FFTF Metal Fuel Testing | 3,800,000 |
| Core Demonstration Experiment (CDE) | 1,000,000 |
| International Collaboration | 500,000 |

## OFFICE OF NUCLEAR ENERGY (Continued)

| | FY 1990 |
|---|---|
| Office of Space and Defense Power Systems | $1,335,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 890,000 |
| Development of Improved Thermoelectric Materials for Space Nuclear Power Systems | 300,000 |
| Development of an Improved Process for the Manufacture of DOP-26 Tridium Alloy Blanks and Exploratory Alloy Improvement Studies | 590,000 |
| Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization | 0 |
| Device or Component Fabrication, Behavior or Testing | $ 110,000 |
| Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices | 110,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 335,000 |
| Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials | 150,000 |
| Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material | 185,000 |
| Office of Naval Reactors | $77,000,000* |

*Approximate

## OFFICE OF NUCLEAR ENERGY

The Office of Nuclear Energy conducts materials research and development through 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 Uranium Enrichment

The Department of Energy is authorized by the Atomic Energy Act of 1954, as amended, to provide toll uranium enrichment services. Customers deliver natural uranium containing about 0.7 percent uranium 235 to one of DOE's plants and, for a fee, DOE returns material enriched to 2-5 percent in the isotope uranium 235 for use in nuclear power reactors. 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 worldwide commercial and United States defense customers to help ensure our national and energy security in an economical, reliable, safe, secure, and environmentally acceptable manner and also to assure a reasonable recovery of the Government's investment.

Revenues received by DOE for the enrichment of uranium are retained and used for the specific purposes of offsetting costs incurred by the Department in providing uranium enrichment service activities as authorized by Section 201 of Public Law 95-238, not withstanding the provisions of Section 3617 of the Revised Statutes (31 USC 484). The sum appropriated is reduced as uranium enrichment revenues are received during a fiscal year so as to result in no net fiscal year appropriations. Total obligations for all uranium enrichment activities in FY 1990 was approximately $1.4 billion.

Presently, uranium is enriched in gaseous diffusion plants that force uranium hexafluoride ($UF_6$) gas through porous barriers. These plants are located at Portsmouth, Ohio, and Paducah, Kentucky. A diffusion plant at Oak Ridge, Tennessee, used since World War II, was placed in standby in 1985 and shut down in 1987. In 1982 and 1985, the DOE determined that of all the new and competing processes the Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS) process had and still has the best potential for providing the lowest cost uranium enrichment in the future.

The U-AVLIS process is based on utilizing differences in the electronic spectra of the 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 in a separator using electromagnetic methods. Collection of the metal product is as a liquid that is allowed to solidify upon withdrawal.

Materials R&D activities within the Office of Uranium Enrichment are varied and, for the most part, classified Restricted Data. In FY 1990, approximately $20.5 million was used in these endeavors and about $25 million is planned for FY 1991. Paragraph summaries of these activities are presented in the second part of this report. The DOE contact is A. P. Litman, (301) 353-5777.

Gaseous Diffusion

Device or Component Fabrication, Behavior or Testing

249. 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.

250. Gaseous Diffusion: Materials and Chemistry Support

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

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

251. U-AVLIS: Separator Materials

- Selection and testing of alternative candidate structural and component materials and coatings for the U-AVLIS separator system.
- Fabrication of full size separator components and subsystems for verification tests.
- Off line operation of full size separator.

252. U-AVLIS: Uranium Processing

- Experiments and design studies on alternatives for preparation of U-AVLIS feed from uranium ore and selection of a baseline process.
- Design of a demonstration system for U-AVLIS metal product conversion to precursor oxide for light water power reactor fuel.
- Interaction with converter, metal maker, and fuel fabricator industries to assure integration into the nuclear fuel cycle.

Office of Civilian Reactor Development

Office of Advanced Reactor Programs

Division of High Temperature Gas-Cooled Reactors

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

Materials Preparation, Synthesis, Deposition, Growth or Forming

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

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

Materials Properties, Behavior, Characterization or Testing

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

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

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

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

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

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

257. Graphite Development and Testing - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact T. D. Burchell, (615) 576-8595

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

258. Metals Technology Development - DOE Contact J. E. Fox, (301) 353-3985; GA Technologies Contact R. F. Turner, (619) 455-2306

- Characterize and qualify the metallic materials selected for application in the near-term steam cycle/cogeneration HTGR system.

- Develop base technology required for design validation and code qualifications.

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

- Selection, characterization, and qualification of high temperature alloys; evaluation of effects of exposures in simulated environments on mechanical properties (creep, fatigue, fracture mechanics).

- Development of the database and correlations required for qualification.

260. Advanced Gas Reactor Materials Development - DOE Contact J. E. Fox, (301) 353-3985; ORNL Contact O. F. Kimball, (615) 574-8258

- Testing and evaluation of high temperature alloys for effects of exposure in simulated reactor environments on mechanical properties.

- Generation of database for development of design criteria and code qualification rules for temperatures above 760°C (1400°F).

Office of Technology Support Programs (LMRs)

The applied research and development technology activities, conducted at several national laboratories, industrial organizations, universities, and through bilateral and trilateral technology programs and exchanges with foreign nations, relate to current and advanced reactor systems. The scope of these activities include the following areas: fuel cycles; design and performance of high quality core components for fuels, blanket, and control systems; development of the structural materials used in these components and systems; development and demonstration of equipment, processes, and procedures for fabricating, processing, handling, and producing mixed oxide bearing fuels, binary and ternary metal fuels, materials, and components; sodium technology; standards and quality assurance; assuring a reliable high quality economical fuel supply for LMRs; destructive and nondestructive testing, examination, and evaluation of core components and the facilities and capabilities for conducting such examinations; responsibility for engineering and supporting facilities; associated safety, safeguards, and nonproliferation; maintaining competent capabilities in the several contractor organizations that conduct the pertinent R&D activities and programs. These activities are responsive to the administration's policies and goals and, to the DOE programs that support them.

In-reactor and out-of-reactor property evaluations are being conducted on core materials, clad/ducts, fuels and absorber materials. Through irradiation testing in FFTF and EBR-II, the Technology Support Programs are developing, qualifying, and verifying the use of reference, improved and advanced mixed oxide and metal fuels and boron carbide absorbers, including full-size driver and blanket fuels, and absorber element pins and assemblies—same for carbide fuels. Fabrication development, evaluation, qualification, and verification (raw material processing, melting, hot working, cold working, and finishing) are conducted on reference, improved, and advanced alloys including in-reactor qualification of pins, ducts, and assemblies. Improved and advanced materials are being tested for use in future cores. The testing for these programs is primarily conducted at government laboratories: Argonne National Laboratory at Chicago, Illinois and Idaho Falls, Idaho; Oak Ridge National Laboratory at Oak Ridge, Tennessee; and Westinghouse Hanford Company at Richland, Washington.

Fuels and Core Materials

Materials Properties, Behavior, Characterization or Testing

261. Fuel Performance Demonstration - DOE Contact Andrew C. Millunzi, (301) 353-3405/FTS 233-3405; ANL Contact Leon C. Walters, (208) 526-7384/FTS 583-7384

- Develop and demonstrate U-Pu-Zr ternary fuel clad with ferritic steel alloy HT-9 or austenitic stainless steel alloy D-9 to at least 150,000 MWD/T burnup.

262. Pyroprocess Development - DOE Contact Eli I. Goodman, (301) 353-2966/FTS 233-2966; ANL Contact James E. Battles, (312) 972-4538/FTS 972-4538

- Develop and demonstrate a pyroprocess that includes electrorefining of binary (U-Zr) and ternary (U-Pu-Zr) metal fuel for recycle in the Integrated Fast Reactor (IFR) and process waste treatment.

263. Fuel Safety Experiments and Analysis - DOE Contact Philip B. Hemmig, (301) 353-3579/FTS 233-3579; ANL Contact John Marchaterre, (312) 972-4561/FTS 972-4561

- Conduct TREAT tests on irradiated ternary metal fuels on U-Pu-Zr to demonstrate safety performance of metallic fuel in fast reactor systems.

264. Core Design Studies - DOE Contact Philip B. Hemmig, (301) 353-3579/FTS 233-3579; ANL Contact D. C. Wade, (312) 972-4858/FTS 972-4858

- Conduct metallic fuel core designs for advanced innovative liquid metal reactors. Evaluate core reactivity coefficients and neutronics performance and actinide self-consumption in closed fuel cycle. Support conversion of oxide fuel core to metal fuel in EBR-II and develop optimized metal fuel core designs for advanced LMR systems.

265. Fuel Cycle Studies - DOE Contact Eli I. Goodman, (301) 353-2966/FTS 233-2966; ANL Contact M. J. Lineberry, (312) 972-7434/FTS 972-7434

- Program will develop equipment for remotized in-cell application, including reusable mold concept for injection-casting furnace, semi-automated pin processor and engineering-scale pyroprocessing equipment for the ultimate commercial fuel cycle facility design and costs.

266. LMR Technology R&D - DOE Contacts Philip B. Hemmig, (301) 353-3579/FTS 233-3579 and C. Chester Bigelow (Seismic), (301) 353-4299/FTS 233-4299; ANL Contact D. C. Wade, (312) 972-4858/FTS 972-4858

- Continue seismic analyses and test support for design.

Structural Materials and Design Methodology

Materials, Properties, Behavior, Characterization and Testing

267. Structural Design/Life Assurance Technology - DOE Contact Andrew C. Milunzi, (301) 353-3405/FTS 233-3405; ORNL Contact Jim Corum, (615) 574-0718/FTS 624-0718

- Develop the structural design methods and criteria for use of modified 9 Cr-1 Mo steel in liquid metal reactor environment. It has been closed out in FY 1989. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

268. Modified 9 Cr-1 Mo Steel Design Properties - DOE Contact Andrew C. Millunzi, (301) 353-3405/FTS 233-3405; ORNL Contact Phil Rittenhouse, (615) 574-5103/ FTS 624-5103

- Conduct long-term creep-rupture tests on base metal, weldments, castings and effects of long-term (up to 10 years) thermal aging on tensile and toughness behavior of modified 9 Cr-1 Mo steel. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

269. MOTA Fabrication and Operation - DOE Contact Andrew C. Millunzi, (301) 353-3405/ FTS 233-3405; WHC Contact Ray J. Puigh, (509) 376-3766/FTS 444-3766

- Fabricate MOTA test train and vehicle to irradiate and test materials, HT-9, Dispersion Strengthened Ferritic Steel (DSF) and others, in a controlled environment in FFTF.

270. Absorber Development - DOE Contact C. Chester Bigelow, (301) 353-4299/ FTS 233-4299, Andrew C. Mullunzi, (301) 353-3405/FTS 233-3405; WHC Contact Alan E. Waltar, (509) 376-5514/FTS 444-5514

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

271. FFTF Metal Fuel Testing - DOE Contact Andrew C. Millunzi, (301) 353-3405/ FTS 233-3405; WHC Contact Alan E. Waltar, (509) 376-5514/FTS 444-5514

- Conduct metal fuel (MFF-2) irradiation testing in FFTF, transient testing in TREAT with HT-9 clad to support conversion of the ALMR from an oxide-fuel core to a binary U-Zr fuel core.

272. Core Demonstration Experiment (CDE) - DOE Contact Jacob Glatter, (301) 353-3921/FTS 233-3921; WHC Contact Alan E. Waltar, (509) 376-5514/ FTS 444-5514

- Complete CDE irradiation in FFTF to extend the fuel lifetime to 1,200 EFPD.

- Evaluate high exposure HT9 data.

273. International Collaboration - DOE Contact Jacob Glatter, (301) 301-353-3921/ FTS 233-3921; WHC Contact Alan E. Waltar, (509) 376-5514/FTS 444-5514

- Complete DSF-1 fuel test with cladding types agreed to with DOE and PNC.
- Complete monitoring irradiation performance in FFTF of PNC fuel (MFA-1 and -2) and blanket (MBA-1) assemblies.
- Characterize and report on production lots of MA-957 cladding.

Office of Space and Defense Power Systems

The Office of Space and Defense Power Systems responsibilities include the development, system safety and production of radioisotope powered thermoelectric generators (RTG) and dynamic power systems for NASA and DOD space and terrestrial applications and advancing base technologies for these power systems. Thus, applied materials research programs are supported in the areas of thermoelectric materials and devices, high temperature heat source materials, materials systems compatibility and safety related materials characterization and testing.

Materials Preparation, Synthesis, Deposition, Growth or Forming

274. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems - DOE Contact W. Barnett, (303) 353-3097; Iowa State University, Ames Laboratory Contact B. Beaudry, (515) 294-1366

- Continue the development of the mechanical alloying process for the development 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, from 300-1000°C of $0.8 \times 10^{-3}/°C$ for "P" type and $1.2 \times 10^{-3}/°C$ for "P" type materials.

275. Development of an Improved Process for the Manufacture of DOP-26 Iridium Alloy Blanks and Exploratory Alloy Improvement Studies - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact E. K. Ohriner, (615) 574-8519

- Development of a consumable arc melt/extrusion route process for the production of DOP-26 iridium alloy sheet and foil. Improve product quality and yield and scaleup size of units processed.
- Exploratory studies of alternate dopants (replace 350-90 PPM thorium in DOP-26 alloy).

276. Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact R. L. Beatty, (615) 574-4536

- Improve process control systems, optimization of process parameters, and accommodate a new type carbon fiber for the manufacture of CBCF, carbon bonded carbon-fiber thermal insulation.

Device or Component Fabrication, Behavior or Testing

277. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact B. E. Foster, (615) 574-4837

- Develop and apply state-of-the-art nondestructive examination (NDE) techniques for Si-Ge thermoelectric materials, multicouple devices and multicouple subassemblies.

Materials Properties, Behavior, Characterization or Testing

278. Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials - DOE Contact W. Barnett, (303) 353-3097; Iowa State University Contact B. Beaudry, (515) 294-1366

- Evaluation and characterization of state-of-the-art Si-Ge/GaP and other "improved" silicon-germanium type thermoelectric materials.

- Evaluate materials compatibility and stability for the MOD-RTG materials systems.

279. Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material - DOE Contact W. Barnett, (303) 353-3097; ORNL Contact M. Martin, (615) 574-4351

- Identify and procure carbon-carbon composite of Graphite Impact Shell dimensions having "cylindrical" reinforcement architecture for evaluation as replacement for current AVCO 3DCC fine weave pierced fabric (orthogonal reinforcement architecture).

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 $88 million in FY 1990 including approximately $48 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Robert H. Steele, (703) 603-5565/FTS 283-5565.

## OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

| | FY 1990 |
|---|---|
| Office of Civilian Radioactive Waste Management - Grand Total | $12,640,100 |
| Office of Civilian Radioactive Waste Management/ Yucca Mountain Site-Characterization Project Office (OCRWM/YMPO) | $12,640,100 |
| Materials Properties, Behavior, Characterization or Testing | $11,074,900 |
| Waste Package Environment | 1,663,000 |
| Waste Form Testing | 3,463,900 |
| Metal Barrier Testing | 1,953,500 |
| Other Engineered Barrier/Waste Package Components | 0 |
| Integrated Testing | 1,950,400 |
| Waste Package: Performance Assessment | 986,500 |
| Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix | 1,057,600 |
| Device or Component Fabrication, Behavior or Testing | $1,565,200 |
| Waste Package: Design, Fabrication and Prototype Testing | 697,700 |
| Waste Package Environmental Field Tests | 867,500 |

# OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

Office of Civilian Radioactive Waste Management/Yucca Mountain Site-Characterization Project Office (OCRWM/YMPO)

The primary goal of the OCRWM/YMPO materials program is the development of tuff-specific waste packages that meet the NRC's performance requirements. This work includes the definition of physical and chemical conditions of the site, evaluation of the package materials, waste package design and performance assessment, prototype waste package fabrication, and performance testing. (As a result of the Nuclear Waste Policy Act Amendments, the Salt Repository Project and the Basalt Waste Isolation Project were terminated effective March 1989.)

Materials Properties, Characterization or Testing

280. Waste Package Environment - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Characterize the time-dependent behavior of the waste environment to establish package design parameters and materials testing conditions, and allow performance analysis.

281. Waste Form Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Perform the testing and evaluation necessary to identify the waste package components required by specific host rock and to select the materials for those components.

- Characterize the behavior of and determine the radionuclide release rates for various waste forms.

282. Metal Barrier Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Characterize behavior of the metal barrier and determine corrosion rates and corrosion mechanisms, including interaction with the environment.

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

283. Other Engineered Barrier/Waste Package Components - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

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

284. Integrated Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

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

285. Waste Package: Performance Assessment - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

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

286. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

- Further develop the geochemical modeling code EQ3/6 for use in long-term predictions for site suitability and radionuclide release from a nuclear waste repository.

Device or Component Fabrication, Behavior or Testing

287. Waste Package: Design, Fabrication and Prototype Testing - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

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

288. Waste Package Environmental Field Tests - DOE Contact C. P. Gertz, (702) 794-7920; LLNL Contact David Short, (415) 422-1287

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

- Determine the responses of tuff to excavation of an underground facility in order to evaluate effects of the heat released by the waste on the hydrologic behavior and effects on components of the engineered barrier system.

## OFFICE OF DEFENSE PROGRAMS

| | FY 1990 |
|---|---|
| Office of Defense Programs - Grand Total | $42,761,000 |
| Office of Research and Advanced Technology | $42,761,000 |
| Research and Technology Development Division | $42,761,000 |
| Sandia National Laboratories - Albuquerque | $16,282,000 |
| Solid State Sciences Directorate, 1100 | $ 8,770,000 |
| Ion Solid Interactions and Surface Sciences Research Department, 1110 | $ 1,370,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 1,370,000 |
| Ion Implantation Studies for Friction, Wear and Microhardness | 300,000 |
| Silicon-Based Radiation Hardened Microelectronics | 670,000 |
| Surface Science | 400,000 |
| Laser and Chemical Physics Research Department, 1120 | $ 1,650,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 1,650,000 |
| Plasma Etching | 500,000 |
| Plasma-Enhanced Chemical Vapor Deposition | 100,000 |
| Laser-Controlled Etching and Deposition of Materials | 250,000 |
| Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy | 300,000 |
| Metallorganic Chemical Vapor Deposition | 500,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Compound Semiconductor and Device Research Department, 1140 | $ 2,000,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 2,000,000 |
| Materials Growth by Molecular Beam Epitaxy (MBE) | 500,000 |
| Materials Growth by MOCVD | 400,000 |
| Strained Layer Superlattices for IR Detectors | 300,000 |
| Novel Processing Technology for Semiconductor Technologies | 500,000 |
| Thin Film Superconductors | 300,000 |
| Condensed Matter Research Department, 1150 | $ 3,000,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 3,000,000 |
| Superconductivity | 650,000 |
| Shock Physics and Chemistry | 500,000 |
| Semiconductors | 600,000 |
| Surface Science | 650,000 |
| Disordered Materials | 600,000 |
| Optoelectronics and Microsensor Research Department, 1160 | $ 750,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 750,000 |
| New Concepts in Microsensors | 750,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Materials and Process Sciences, 1800 | $ 7,512,000 |
| Organic and Electronic Materials Department, 1810 | $ 2,145,000 |
| Chemistry of Organic Materials Division, 1811 | $ 475,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 100,000 |
| Sulfonated Aromatic Polysulfones | 100,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 175,000 |
| Radiation Hardened Dielectrics | 50,000 |
| Organic Nonlinear Optical Materials | 125,000 |
| Physical Chemistry and Mechanical Properties of Polymers Division, 1812 | $ 455,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 130,000 |
| Chemistry of Plasma Etching and Deposition Processes | 130,000 |
| Materials Structure and Composition | $ 325,000 |
| Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy | 75,000 |
| Mechanistic and Kinetic Studies of Polymer Aging | 250,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Physical Properties of Polymers Division, 1813 | $ 351,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 180,000 |
| Microporous Foam Development | 150,000 |
| Development of Removable Encapsulants | 30,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 71,000 |
| Mechanical Properties of Encapsulants | 21,000 |
| Deformation of Kevlar Fabrics | 50,000 |
| Materials Structure and Composition | $ 100,000 |
| Theory of Polymer Dynamics | 100,000 |
| Electronic Property Materials Division, 1815 | $ 864,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 864,000 |
| Nonlinear Optical Materials | 100,000 |
| Hydrogen Effects in Silicon | 50,000 |
| Ferroelectric Thin Films for Nonvolatile Memories | 200,000 |
| Sensor Fabrication from Porous Silicon Using Electrochemical Techniques | 77,000 |
| Improved Chemometric Techniques | 95,000 |
| Direct Bonding of Films and Substrate Using Ion Processing | 59,000 |
| Kinetics of the Oxidation of Solder Alloys | 59,000 |
| Segregation of Impurities to Defects in Silicon | 54,000 |
| Characterization of Semiconductor Materials | 120,000 |
| Support for Advanced Component Research | 50,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Materials and Environmental Sciences Department, 1820 | $ 205,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 205,000 |
| Gamma Imaging of Radioactive Waste | 84,000 |
| Diamond Coating | 49,000 |
| Phase Transformation in Thin Ferroelectric Films | 72,000 |
| Metallurgy Department, 1830 | $ 1,462,000 |
| Physical and Joining Metallurgy Division, 1831 | $ 425,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 425,000 |
| Weldability of Alloys | 125,000 |
| Segregation Behavior During Solidification of Alloys | 50,000 |
| Solid State Reactions Between Metal Substrates and Solders | 100,000 |
| Fluxless Soldering | 50,000 |
| Weld Process Development | 100,000 |
| Packaging and Structural Metallurgy Division, 1832 | $ 503,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 60,000 |
| Solid Film Lubrication Studies | 60,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Packaging and Structural Metallurgy Division, 1832 (continued) | |
| Materials Properties, Behavior, Characterization or Testing | $ 443,000 |
| Wear Modeling of Ceramics | 77,000 |
| Wetting and Mechanical Behavior of Interfacial Intermetallics in Solder Joints | 52,000 |
| Stress Corrosion Cracking - Modeling 2-D Crack Growth | 77,000 |
| Al-Cu Thin Film Studies | 37,000 |
| Stress Voiding in Aluminum Metallizations | 200,000 |
| Melting Research and Solder Processing Division, 1833 | $ 280,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 200,000 |
| Investment Casting | 80,000 |
| Plasma Spraying | 120,000 |
| Device or Component Fabrication, Behavior or Testing | |
| Laser Welding | 80,000 |
| Corrosion, Cleaning, and Thin Film Technology Division, 1834 | $ 254,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 63,000 |
| Development of Multilayer Metallizations | 63,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Corrosion, Cleaning, and Thin Film Technology Division, 1834 (continued) | |
| Materials Properties, Behavior, Characterization or Testing | $ 133,000 |
| Corrosion of Aluminum Metallization on Microelectronics | 50,000 |
| Characterization of Diamond Films for Tribological Applications | 83,000 |
| Device or Component Fabrication, Behavior or Testing | $ 58,000 |
| Development of Fiber-Optic Metallization for Joining | 58,000 |
| Chemistry and Ceramics Department, 1840 | $ 3,700,000 |
| Interfacial Chemistry and Coating Research Division, 1841 | $ 500,000 |
| Electronic Ceramics Division, 1842 | $ 500,000 |
| Ceramics Development Division, 1845 | $ 550,000 |
| Inorganic Meterials Chemistry Division, 1846 | $ 2,150,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 750,000 |
| Electrolytic and Electrophoretic Methods for Materials Processing | 50,000 |
| Aerosol Production of Fine Ceramic Powders | 50,000 |
| Chemically Prepared Ceramic Films for Opto-electronic Applications | 200,000 |
| Development of New Glasses and Glass-Ceramics | 250,000 |
| Preparation of Ceramic Powders by Chemical Techniques | 200,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Albuquerque (continued) | |
| Inorganic Meterials Chemistry Division, 1846 (continued) | |
| Materials Structure and Composition | $ 400,000 |
| Structure of Novel Glasses | 200,000 |
| Structure of Sol-Gel Films | 200,000 |
| Materials Properties, Behavior, Characterization and Testing | $ 700,000 |
| Molecular Beam Studies of Hydrogen in Metals | 200,000 |
| Electronic Ceramics | 200,000 |
| Ceramic Fracture | 100,000 |
| Reactivity and Bonding of Glasses and Ceramics to Metals | 200,000 |
| Device or Component Fabrication, Behavior or Testing | $ 300,000 |
| Sensor Development | 100,000 |
| SAW Development | 200,000 |
| Sandia National Laboratories - Livermore | $ 2,900,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 1,050,000 |
| Powder Metallurgy | 200,000 |
| Advanced Electrodeposition Studies | 300,000 |
| Metal Forming | 100,000 |
| Advanced Foam Materials | 200,000 |
| Tritium Getter Technology | 50,000 |
| Plasma Processing | 200,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Sandia National Laboratories - Livermore (continued) | |
| Materials Properties, Behavior, Characterization or Testing | $ 1,350,000 |
| Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys | 500,000 |
| Joining Science and Technology | 400,000 |
| Composites: Characterization and Joining | 200,000 |
| Compatibility, Corrosion, and Cleaning of Materials | 50,000 |
| Helium in Metal Tritides | 200,000 |
| Instrumentation and Facilities | $ 500,000 |
| Tritium Facility Materials Characterization and Testing | 300,000 |
| New Analytical Techniques | 100,000 |
| New High Resolution Electron Microscopy Facility | 100,000 |
| Lawrence Livermore National Laboratory | $11,047,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 1,940,000 |
| Inorganic Aerogels | 350,000 |
| Photoactivated Catalysis on Aerogels | 200,000 |
| Organic Aerogels | 200,000 |
| Polymer Materials Development and Coating | 1,000,000 |
| Atomic Engineering | 190,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Lawrence Livermore National Laboratory (continued) | |
| Materials Structure and Composition | $ 1,795,000 |
| Theory of the Structure and Dynamics of Molecular Fluids | 300,000 |
| Plutonium Pyrochemical Research | 25,000 |
| Electronic Structure in Superconducting Oxides | 1,290,000 |
| Electronic Structure Study of the Thermodynamic and Mechanical Properties of Al-Li Alloys | 180,000 |
| Materials Properties, Behavior, Characterization or Testing | $ 5,727,000 |
| Nuclear Spin Polarization | 1,100,000 |
| Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures | 90,000 |
| Pretransformation Behavior in Alloys | 500,000 |
| The Structure Property Link in Sub-Nanometer Materials | 60,000 |
| Synchrotron Radiation-Based Materials Science | 800,000 |
| Structural Transformation and Precursor Phenomena | 150,000 |
| Underwater Explosive Energetics | 150,000 |
| Composite Explosive Energetics | 150,000 |
| Low Vulnerability Explosives | 420,000 |
| Fundamentals of Explosive Vulnerability | 400,000 |
| Very High Energy Density Materials | 50,000 |
| Use of Finite Element Analysis to Understand Delayed Failure in Silver-Interlayer Welds | 100,000 |
| Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain | 100,000 |
| Theoretical and Experimental Studies of Solid Combustion Reactions | 100,000 |
| Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides | 175,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | |
|---|---|
| | FY 1990 |
| Lawrence Livermore National Laboratory (continued) | |
| Materials Properties, Behavior, Characterization or Testing (continued) | |
| Oxidation and Liquid Metal Resistant Coatings | 70,000 |
| Development of Ultrafine Microstructures Through Rapid Solidification Rate Processing | 90,000 |
| Failure Characterization of Composite Materials | 330,000 |
| Modeling Superplastic Materials | 260,000 |
| Creep Model for Fiber Reinforced Epoxy-Resin Composites | 58,000 |
| Superplastic Flow of Ceramics and Intermetallics | 125,000 |
| Structural Joints for Composite Materials | 69,000 |
| Interfaces, Adhesion and Bonding | 380,000 |
| Device or Component Fabrication, Behavior or Testing | $ 945,000 |
| IC Protective Coatings | 720,000 |
| Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography | 50,000 |
| Optical Diagnostics of High Explosives Reaction Chemistry | 175,000 |
| Instrumentation and Facilities | $ 640,000 |
| Scanning Tunneling Microscopy | 320,000 |
| Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector | 320,000 |
| Tritium Facility Upgrade | (7,800,000)* |
| Decontamination and Waste Treatment Facility (DWTF) | (7,700,000)* |

*Line-item construction projects. They are not included in subtotal or total.

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Los Alamos National Laboratory | $12,532,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $ 6,440,000 |
| Actinide Processing Development | 1,350,000 |
| Plutonium Oxide Reduction | 150,000 |
| Ion-Beam Implantation | 200,000 |
| Electroplating Low Atomic Number Materials | 100,000 |
| Liquid Crystal Polymer Development | 300,000 |
| Low-Density, Microcellular Plastic Foams | 250,000 |
| Target Coatings | 400,000 |
| Physical Vapor Deposition and Surface Analysis | 700,000 |
| Chemical Vapor Deposition (CVD) Coatings | 200,000 |
| Polymers and Adhesives | 450,000 |
| Tritiated Materials | 511,000 |
| Salt Fabrication | 379,000 |
| Slip Casting of Ceramics | 150,000 |
| Glass and Ceramic Coatings | 40,000 |
| Cold Pressing, Cold Isostatic Pressing and Sintering | 10,000 |
| Plasma-Flame Spraying Technology | 185,000 |
| Rapid Solidification Technology | 100,000 |
| Microwave Sintering/Processing | 120,000 |
| Predictions of Super Strong Polymers | 565,000 |
| Synthesis of Ceramic Coatings | 30,000 |
| Laser Surface Treatment of Materials | 250,000 |
| Materials Structure or Composition | $ 1,187,000 |
| Actinide Surface Properties | 700,000 |
| Neutron Diffraction of Pu, Pu Alloys and Other Actinides | 237,000 |
| Surface, Material and Analytical Studies | 250,000 |

## OFFICE OF DEFENSE PROGRAMS (Continued)

| | FY 1990 |
|---|---|
| Los Alamos National Laboratory (continued) | |
| Materials Properties, Behavior, Characterization or Testing | $ 2,625,000 |
| Mechanical Properties of Plutonium and Its Alloys | 450,000 |
| Phase Transformation in Pu and Pu Alloys | 450,000 |
| Plutonium Shock Deformation | 350,000 |
| Non-Destructive Evaluation | 500,000 |
| Powder Characterization | 50,000 |
| Shock Deformation in Actinide Materials | 200,000 |
| Dynamic Mechanical Properties of Weapons Materials | 225,000 |
| Dynamic Testing of Materials for Hyper-Velocity Projectiles | 100,000 |
| Mechanical Properties | 300,000 |
| Device or Component Fabrication, Behavior or Testing | $ 2,280,000 |
| Radiochemistry Detector Coatings | 200,000 |
| Target Fabrication | 1,500,000 |
| Filament Winder | 80,000 |
| Polymeric Laser Rods | 150,000 |
| High Energy Density Welding in Hazardous Environments | 350,000 |

# 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, analysis and coordination of international activities related to nuclear technology and materials, and the management of waste from defense program activities.

Materials activities in Defense Programs are concentrated in the Office of Research and Advanced Technology and in the Office of Nuclear Materials Production. Within the Office of Research and Advanced Technology, materials activities are supported by the Inertial Fusion Division and by the Research and Technology Development Division. The bulk of these activities are performed at the three weapons program national laboratories: Sandia, Lawrence Livermore, and Los Alamos.

## Office of Research and Advanced Technology

## Research and Technology Development Division

## Sandia National Laboratories - Albuquerque

## Solid State Sciences Directorate, 1100

## Ion Solid Interactions and Surface Sciences Research Department, 1110

The mission of Department 1110 is to provide Sandia National Laboratories with a comprehensive research program and technology base in ion implantation, ion-solid microanalysis/channeling thin film kinetics and epitaxy, and defects and hydrogen in solids. The research is designed to enhance fundamental understanding of the physical and chemical processes necessary to control the near-surface and interfacial regions of solids as well as to develop new techniques for the controlled synthesis, modification and analysis of these near-surface and interfacial regions. A major aspect of the work is thus to develop an underlying understanding and control of thin film kinetics, epitaxy, defects, hydrogen-materials interactions, alloying processes, and the formation of metastable and amorphous phases. In addition, the mission of the department is to relate this knowledge to laboratory problems and needs in the development of advanced weapons and energy systems.

Materials Properties, Behavior, Characterization or Testing

289. Ion Implantation Studies for Friction, Wear and Microhardness - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts D. M. Follstaedt, (505) 844-2102, S. M. Myers, (505) 844-6076 and L. E. Pope, (505) 844-5041

- Ion implantation is used to modify the surface and near-surface regions of metals and these implantation-modified materials are evaluated for their improved friction and wear characteristics.

290. Silicon-Based Radiation Hardened Microelectronics - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contacts H. J. Stein, (505) 844-6279, K. L. Brower, (505) 844-6131 and J. A. Knapp, (505) 844-2305

- Optical, electrical and compositional measurements, in conjunction with electron paramagnetic resonance and related techniques are used to determine the fundamental defect structures and materials properties required for radiation-hardened Si-based microelectronics.

291. Surface Science - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact T. A. Michalski, (505) 844-5829

- Scanning tunneling microscopy, field ion microscopy, Auger electron spectroscopy, UV photoemission spectroscopy, and thermal desorption are being used to study the early stages of epitaxy, oxidation and corrosion of metals and semiconductors and adhesion of polymers to metals.

- Novel chemical vapor deposition techniques are being developed to produce more uniform and reliable multicomponent pyrotechnics.

Laser and Chemical Physics Research Department, 1120

Materials processing science studies emphasizing chemical vapor deposition and plasma- and photo-enhanced vapor deposition and etching are carried out. Emphasis is on microelectronic and optoelectronic materials and processing methods. Examples of ongoing studies are provided below.

Materials Properties, Behavior, Characterization or Testing

292. Plasma Etching - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contacts K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

- Fundamental studies of plasmas of the type widely used in the manufacture of large-scale and very-large-scale integrated electronic circuits to etch small features in semiconductors, dielectrics and conductors.
- Emphasis is on new process methods and methodologies for improved pattern-transfer fidelity with less damage to the underlying material, and on process monitors that may lead to improved process reliability.

293. Plasma-Enhanced Chemical Vapor Deposition - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contacts K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

- Fundamental studies of plasma-enhanced chemical vapor deposition, PECVD, aimed at processes that give higher quality materials having good adhesion to the underlying structure.
- *In situ* monitors for process control.

294. Laser-Controlled Etching and Deposition of Materials - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact A. Wayne Johnson, (505) 844-8782

- Study of the technological limits of laser-controlled deposition and etching of conductors and insulators on microelectronic circuits.
- Potential applications in the correction of design errors in prototype circuits and the customization of large-scale integrated circuits.

295. Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact J. R. Creighton, (505) 844-3955

- Study of the primary chemical surface reactions of organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc.) used as sources of elemental constituents for the growth of compound semiconductors.
- Application of such techniques as metallorganic chemical-vapor deposition (MOCVD), chemical-beam epitaxy (CBE), and atomic layer epitaxy (ALE).

296. Metallorganic Chemical Vapor Deposition - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contacts K. P. Killeen, (505) 844-5164 and M. E. Coltrin, (505) 844-7843

- Theoretical modelling of the fluid dynamics and both the volume and the surface chemistry, together with application of *in situ* measurement tools to gain new insight into the underlying physics and chemistry of the MOCVD process.

- Goals of this work are the development of processes and process control procedures that yield higher quality materials and more abrupt heterointerfaces, and identification of chemical precursors that are less toxic and otherwise more safe to handle.

Compound Semiconductor and Device Research Department, 1140

Study and application of semiconductor strained-layer superlattices and heterojunction materials to explore solutions to new and existing semiconductor materials problems, by coordination of semiconductor physics (theory and experiment) and materials science. This program investigates fundamental material properties including band structure, electronic transport, crystal stability, and linear and nonlinear optical properties. It also includes investigation of thin film high temperature superconductors for hybrid compound semiconductor/superconductor applications. The materials under study have a wide range of applications for high speed and microwave technology, optical detectors, lasers, and optical modulation and switching.

Materials Preparation, Synthesis, Deposition, Growth or Forming

297. Materials Growth by Molecular Beam Epitaxy (MBE) - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts L. R. Dawson, (505) 846-3451, T. M. Brennan, (505) 844-3233 and J. F. Klem, (505) 844-9102

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

298. Materials Growth by MOCVD - DOE Contact C. B. Hilland, (301) 353-3687/ FTS 233-3687; Sandia Contact R. M. Biefield, (505) 844-1556

- Growth of GaP/GaAsP and InAsSb/InSb SLSs for high temperature radiation-hard electronic devices and for long wavelength IR detectors, respectively.
- A primary goal of this effort is to identify suitable dopants for n and p type InAsSb/InSb SLSs.
- A further goal is to fabricate p-n junction photodiodes from these materials for IR detectors in the 8-12 $\mu m$ wavelength region.

299. Strained Layer Superlattices for IR Detectors - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact P. S. Peercy, (505) 844-4309

- Strained layer superlattices based on the InAsSb/InSb and InAsSb/InSb/AlSb systems are being investigated for use as attractive alternatives to the unstable HgCdTe alloys for IR detector applications in the 8-12 $\mu m$ range.
- Growth by both MBE and MOCVD techniques.
- Photovoltaic detector with $D^* > 1 \times 10^{10}$ cm $\sqrt{HZ}/W$ at 10 $\mu m$ and 77K and photoconductive detection to 15 $\mu m$ have been demonstrated.

300. Novel Processing Technology for Semiconductor Technologies - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact D. S. Ginley, (505) 844-8863

- This program involves studies of new technologies for formation of diffusion barriers, Shottky barrier and Ohmic contact formation, passivation layer development, deposition of reactive alloys, and deposition and patterning of high temperature superconductors.

301. Thin Film Superconductors - DOE Contact C. B. Hilland, (301) 353-3687/ FTS 233-3687; Sandia Contact D. S. Ginley, (505) 844-8863/FTS 844-8863

- Thin films of the high temperature superconductors in the Y-Ba-Cu-O and Tl-Ca-Ba-Cu-O systems are being prepared by MBE, E-beam evaporation and sputtering.
- Strongly-linked polycrystalline films with critical currents approaching 1,000,000 $A/cm^2$ at 77K have been demonstrated.
- Patterning and contacting technology for the films for device applications is also being developed.

Condensed Matter Research Department, 1150

The mission of Department 1150 is to provide fundamental understanding and strong technology bases in novel materials and structures, surface physics and shock wave physics and chemistry. Both experimental and theoretical research are performed. Current areas of emphasis include high $T_c$ superconductors, shock-induced solid state chemistry, disordered materials, high temperature semiconducting borides, defects in semiconductors, surface desorption and ferroelectrics.

Materials Properties, Behavior, Characterization or Testing

302. Superconductivity - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact B. Morosin, (505) 844-8169

- Transport, magnetic and structural measurements to access the fundamental factors which limit the performance of ceramic superconductors.
- Development of theoretical models of high temperature superconductivity.
- Development of new processing technologies for ceramic superconductors, in particular high pressure, high temperature oxygen treatments.

303. Shock Physics and Chemistry - DOE Contact C. B. Hilland, (301) 353-3687/ FTS 233-3687; Sandia Contact R. A. Graham, (505) 844-1931

- Both organic and inorganic solids are being investigated to determine the influence of molecular structure on shock-induced bond scission, and the influence of line and point defects on the observed, enhanced, shock-induced solid state reactivity.

- The influence of shock modification on the properties and synthesis of high $T_c$ superconductors is being explored. Shock-activated thermal batteries are being studied to determine the mechanisms and materials parameters which influence electrical output.

- A revolutionary time-resolved dynamic stress gauge using the piezoelectric polymer $PVF_2$ is being developed.

304. Semiconductors - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts D. Emin, (505) 844-3431 and H. P. Hjalmarson, (505) 846-0355

- Theoretical and experimental studies of electronic properties of boron carbide at high temperatures.

- Radiation-induced defects and their deep electronic levels in silicon and compound semiconductors and the role of these defects in device degradation.

- Physics of light-hole devices based on strained layer superlattices.

305. Surface Science - DOE Contact C. B. Hilland, (301) 353-3687; 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.

306. Disordered Materials - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact G. A. Samara, (505) 844-6653

- Application of polymeric synthesis routes to ceramic materials.

- Gas phase materials processing.

- Gelation in foam precursors and sol-gel glasses.

- Fundamentals of film formation.

- The physics and formation of microemulsions.

Optoelectronics and Microsensor Research Department, 1160

The mission of Department 1160 is to provide Sandia National Laboratories with a comprehensive science and technology base in photonics and microsensor research. A fundamental understanding of the interaction of materials with both electromagnetic and mechanical forms of energy as well as their chemical environment are used to facilitate the design of new photonic and sensor devices. Activities include research into advanced materials and devices for optical sources; modulators and detectors; information processing; and chemical sensing.

Materials Properties, Behavior, Characterization or Testing

307. New Concepts in Microsensors - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts R. C. Hughes, (505) 844-8172, A. J. Ricco, (505) 844-4947; M. A. Butler, (505) 844-6897

- Radiation-sensing field-effect transistor (RADFET) which operates by the trapping of radiation-produced holes in the silicon dioxide gate dielectric of the FET.
- Chemical sensors which operate by inducing charged layers at the metal-silicon dioxide interface in response to the chemical species.
- Acoustic wave devices for detection of solid-liquid interface phenomena like viscosity, freezing, and low level chemical detection.
- Optically-based corrosion and energy impulse detectors for high speed impulse detection and remote corrosive species detection.
- A miniature optical fiber micromirror chemical detector that can distinguish between water and common organic solvents.

Materials and Process Sciences, 1800

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

308. Sulfonated Aromatic Polysulfones - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts R. L. Clough, (505) 844-3492, C. Arnold, Jr., (505) 844-8728, and R. A. Assink, (505) 844-6372

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

Materials Properties, Behavior, Characterization or Testing

309. Radiation Hardened Dielectrics - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts R. L. Clough, (505) 844-3492 and C. Arnold, Jr., (505) 844-8728

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

- These materials will be used in capacitors and cables exposed to high dose-rate radiation so that little charge is lost due to RIC in this environment.

- Processing parameters have been optimized.

310. Organic Nonlinear Optical Materials - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts R. L. Clough, (505) 844-3492; P. A. Cahill, (505) 844-5754, G. E. Pike, (505) 844-7562, and M. B. Sinclair, (505) 844-5506

- Research on fabrication of organic nonlinear optical devices on semiconductor substrates has been initiated.

Physical Chemistry and Mechanical Properties of Polymers Division, 1812

Division 1812 develops new organic materials, structurally and chemically characterizes organic materials, and studies their mechanical properties. It is responsible for characterizing the molecular, electronic, and microphase structure of organic materials and their chemical reactivity toward the use environment as well as formulation of organic composites and adhesives.

Materials Preparation, Synthesis, Deposition, Growth or Forming

311. Chemistry of Plasma Etching and Deposition Processes - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts C. L. Renschler, (505) 844-0324 and R. J. Buss, (505) 844-7494

- Study of chemistry of glow discharge plasmas using molecular beam and laser techniques.
- Application to selectivity in etching for microelectronic fabrication.
- Also applied to deposition of films for chemical sensing applications.

Materials Structure and Composition

312. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts C. L. Renschler, (505) 844-0324 and R. H. Assink, (505) 844-6372

- Use of $^{13}C$ and $^{1}H$ spectroscopy of precursor liquids for encapsulants and foams.
- Studies of coal liquefaction catalysts and processes.
- Study of sol-gel kinetics.
- Imaging techniques for liquid and solid foams.

313. Mechanistic and Kinetic Studies of Polymer Aging - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts C. L. Renschler, (505) 844-0324, K. T. Gillen, (505) 844-7494, and R. L. Clough, (505) 844-3492

- Mechanistic studies of thermo-oxidative degradation routes in polymers.
- Development of novel tools and techniques to quantify polymer aging.
- Development of kinetic theory and validation with experimental data.

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

314. Microporous Foam Development - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts J. G. Curro, (505) 844-3963, R. R. Lagasse, (505) 845-8333

- Development of new polymer and carbon foams which have both low density and small cell sizes (0.1 to 10 microns).
- Process utilizes thermally induced phase separation followed by solvent removal steps such as extraction or freeze-drying.

315. Development of Removable Encapsulants - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts J. G. Curro, (505) 844-3963 and P. B. Rand, (505) 844-7953

- Development of removable encapsulant to allow rework of electronic components.
- Polymer beads (with blowing agent) poured into assembly and heated to fuse polymer. Encapsulant removed with solvent.

Materials Properties, Behavior, Characterization or Testing

316. Mechanical Properties of Encapsulants - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts J. G. Curro, (505) 844-3963 and D. B. Adolf, (505) 844-4773

- Measurement of linear elastic properties (coefficient of thermal expansion, bulk modulus, and shear modulus) as functions of temperature that lead to stresses upon thermal cycling for common polymeric encapsulants.
- Future studies will focus on the ultimate properties of these materials for use in determining failure criteria using computer codes.

317. Deformation of Kevlar Fabrics - DOE Contact C. B. Hilland, (301) 353-3687/ FTS 233-3687; Sandia Contacts J. G. Curro, (505) 844-3963 and W. E. Warren, (505) 844-4445

- The effect of specific fabric microstructure and Kevlar yarn properties on the effective elastic properties of the fabric are being investigated theoretically and experimentally to allow optimization of the mechanical properties of parachute fabrics.

Materials Structure and Composition

318. Theory of Polymer Dynamics - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact J. G. Curro, (505) 844-3963

- Extension of Mode-Mode-Coupling Theory to polymeric liquids.
- Calculation of structure-property relationships from first principles, with no adjustable parameters.
- Develop understanding of important length scales, as observed in scattering experiments.

Electronic Property Materials Division, 1815

Division 1815 provides support to Sandia programs through selection, development, and characterization of electronic materials. Responsibilities span exploratory development through design, production, and stockpiling. The Division also performs in-depth studies in order to understand material properties and associated electronic phenomena. Areas of activity include electronic materials, dielectrics, and optical materials.

Materials Properties, Behavior, Characterization or Testing

319. Nonlinear Optical Materials - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contacts G. E. Pike, (505) 844-7562 and M. L. Sinclair, (505) 844-5506

- Optical and electrooptical change of refractive index are being measured for organic molecules and polymers.

320. Hydrogen Effects in Silicon - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts G. E. Pike, (505) 844-7562 and R. A. Anderson, (505) 844-7676

- Kinetics of hydrogenation and dopant passivation in silicon.

- Hydrogen dopant complex dissociation is electronically controlled.

321. Ferroelectric Thin Films for Nonvolatile Memories - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact G. E. Pike, (505) 844-7562 and W. K. Schubert, (505) 846-6548

- Electron spin resonance of thin PZT film to investigate the role of microstructure, impurities and defects in determining ferroelectric performance.

Materials and Environmental Sciences Department, 1820

Department 1820 performs chemical analysis and materials characterization in support of weapon and energy programs and projects throughout the laboratory, and it has responsibility for the development of advanced techniques to meet anticipated needs. In addition, the department is involved in other areas such as materials compatibility, minimizing waste and certain other environmental areas.

Materials Properties, Behavior, Characterization or Testing

322. Gamma Imaging of Radioactive Waste - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact Laura Gilliom, (505) 844-3936 and Willard Hareland, (505) 844-7758

- Two-dimensional imaging capability for high level radioactive waste is being developed to be used in conjunction with robots to characterize DOE wastes stored at various sites.

323. Diamond Coating - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact Laura Gilliom, (505) 844-3936 and D. R. Tallant, (505) 844-3629

- Raman spectroscopy is being used to characterize diamond and diamond-like films prepared in other Sandia laboratories.

324. Phase Transformation in Thin Ferroelectric Films - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact Laura Gilliom, (505) 844-3936 and R. P. Goehner, (505) 844-9200

- X-ray crystallography is being used to determine the phase transformations that occur when an electric field is applied to these materials.

325. Sensor Fabrication from Porous Silicon Using Electrochemical Techniques - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact M. Keenan, (505) 844-2190 and M. Kelly, (505) 844-4031

- Electrochemical techniques are being used to fabricate moisture sensors and to characterize defects in SOI technology. This project is joint with other Sandia organizations.

326. Improved Chemometric Techniques - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact M. Keenan, (505) 844-2190 and D. Haaland, (505) 844-5292

- Application of multivariate analysis to spectral data.
- Application to instrumental analysis of materials with particular emphasis on the identification of outliers and the transfer of the calibration model data from one instrument to another.

327. Direct Bonding of Films and Substrate Using Ion Processing - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact J. Borders, (505) 844-8855 and A. Galuska, (505) 844-3187

- High energy ion mixing used as a tool to better understand the mechanisms of certain thin-film bonding processes and determine improved bonding procedures.

328. Kinetics of the Oxidation of Solder Alloys - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact J. Borders, (505) 844-8855 and J. Nelson, (505) 846-7388

- Determination of rate of oxide growth on solder material in order to predict long-term reliability of weapon components.

329. Segregation of Impurities to Defects in Silicon - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact M. Carr, (505) 846-1405 and J. R. Michael, (505) 844-9115

- Development of analytical electron microscopy as a tool to analyze the extent to which impurities in silicon migrate to defects.

330. Characterization of Semiconductor Materials - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact M. Carr, (505) 846-1405 and T. Headley, (505) 844-4787

- Application of various analytical instruments to the characterization of semiconductor materials in support of research centered elsewhere in the laboratory.

331. Support for Advanced Component Research - DOE Contact C. B. Hilland, (301) 353-3687; SNL Contact J. Borders, (505) 844-8855

- Application of various analytical instruments to the characterization of materials associated with the development of advanced components centered elsewhere in the laboratory.

Metallurgy Department, 1830

Department 1830 selects, develops, and characterizes all metal based materials and their related manufacturing processes that are required to meet current and future 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 through microstructural interpretation and the modeling of processes, structure, and properties provides the basis for alloy and process development and increases the confidence of behavior predictions.

Physical and Joining Metallurgy Division, 1831

This organization is tasked with developing fundamental understandings of the thermal/chemical interactions which control microstructure and properties in metals and alloys. As such, it will provide expertise in microstructural interpretation, and microstructural evolution of metals and alloys as a result of manufacturing processes, especially welding, brazing, casting, and soldering. Interpretation of solidification and solid state transformations in metal alloys and the modeling and interpretation of diffusive and other kinetic processes are this division's responsibility. Development of phase equilibria and thermodynamic information for metallurgically important systems such as solder alloys and intermetallics will be carried out by personnel in this organization. Weld process research and subsequent implementation at the Production Agencies is also a major responsibility.

Materials Properties, Behavior, Characterization or Testing

332. Weldability of Alloys - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts C. V. Robino, (505) 844-6557, M. C. Maguire, (505) 844-1625, G. A. Knorovsky, (505) 844-1129, and M. J. Cieslak, (505) 845-9144

- Studies of wetting of solder on alloys used in electronic components.

333. Segregation Behavior During Solidification of Alloys - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts C. V. Robino, (505) 844-6557 and M. J. Cieslak, (505) 846-7500

- Study of the distribution of elements following solidification of welds to understand hot-cracking in the region containing these low melting point constituents.
- Diffusion in the solid, solidification in multicomponent systems and non-planar front solidification are being treated.

334. Solid State Reactions Between Metal Substrates and Solders - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts P. T. Vianco, (505) 844-2329 and A. D. Romig, (505) 844-8358

- Integrated experimental and diffusion modeling program investigating reactions between fusible alloy solders, based on Pb, Sn, In, etc., and metallic substrates. Efforts are aimed at determining the stability and formation rates of intermediate phases as a function of temperature.
- Systems currently under study include Au/Pb-In, Au-Pd/Pb-In, Cu/Pb-Sn, Cu/Pb-In, Pd/Pb-In.

335. Fluxless Soldering - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact F. M. Hosking, (505) 844-4925

- Fluxes promote wetting when soldering, but present potential long term reliability problems with respect to the potential for corrosion if their residues are not removed.

- The goal of this work is to find a reactive gas and specific processing conditions which produce solder joints which are comparable to those produced using rosin based fluxes, and are environmentally benign.

336. Weld Process Development - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts P. W. Fuerschbach, (505) 845-8877, G. A. Knorovsky, (505) 844-1129, C. V. Robino, (505) 844-6557, and M. C. Maguire, (505) 844-1625

- Heat input minimization to maximize melting efficiency in gas-tungsten-arc and plasma-arc welding has been quantified and a functional relationship developed which guides optimization of melting for a given material, process, and weld joint design.

- The mechanical response of resistance weld heads has been characterized and its influence on weld processing is being evaluated. A method of *in-situ*, non-destructive evaluation of penetration in laser welding is being developed.

Packaging and Structural Metallurgy Division, 1832

The mission of the Packaging and Structural Metallurgy Division 1832 is to provide the understanding and characterization of the mechanical, friction, and wear properties of materials. 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 Preparation, Synthesis, Deposition, Growth or Forming

337. Solid Film Lubrication Studies - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact M. T. Dugger, (505) 844-1091

- Solid film lubricants are under development for use in very clean environments.

- Available films are being characterized and novel methods of $MoS_2$ deposition will be examined in terms of both productivity and performance.

Materials Properties, Behavior, Characterization or Testing

338. Wear Modeling of Ceramics - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts M. T. Dugger, (505) 844-1091 and R. J. Bourcier, (505) 844-6638

- Develop a model to simulate the wear of ceramic surfaces using fundamental materials properties and the statistical parameters that characterize the surface topography on an appropriate microscopic scale.

- Measure topographical characteristics of actual wear surfaces using atomic force microscopy and use these data to refine and validate the modeling.

339. Wetting and Mechanical Behavior of Interfacial Intermetallic in Solder Joints - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts D. R. Frear, (505) 845-9023 and J. J. Stephens, (505) 845-9209

- Intermetallics play an important role in the formation and mechanical response of solder joints. This program examines the wetting, the growth kinetics, and the resultant mechanical response of several intermetallics of interest in solder applications.

340. Stress Corrosion Cracking - Modelling 2-D Crack Growth - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts R. J. Bourcier, (505) 844-6638 and W. B. Jones, (505) 845-8301

- Microscopic models explain only one dimensional growth of stress corrosion cracks.

- A two dimensional model is being developed to predict the crack growth which occurs in actual specimens. Features such as microstructure and applied stress field are incorporated into the model.

341. Al-Cu Thin Film Studies - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts D. R. Frear, (505) 845-9023 and A. D. Romig, (505) 844-8358

- Investigation of mechanisms for the electromigration resistance of Al-Cu metallizations.

- The microstructure of Al-Cu films will be varied and analytical electron microscopy used to examine the distribution of Cu within the microstructure and its reaction in electromigration testing.

342. Stress Voiding in Aluminum Metallizations - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts J. A. Van Den Avyle, (505) 845-8034, R. J. Bourcier, (505) 844-6638, and F. G. Yost, (505) 844-5446

- The measurement and prediction of stresses in passivated aluminum metallization conductor lines on integrated circuits is key to the prediction of stress voiding.
- Experimental and analytic studies are underway to measure these stresses by X-ray diffraction and to model them using finite element methods.

Melting Research and Solder Processing Division, 1833

This Division supports the laboratories by selecting, characterizing, and developing metallurgical processes needed in the manufacture of components and systems. The objective is to provide process definition and control by understanding the mechanisms which operate. Principal processes currently under study include laser welding, vacuum arc remelting, electroslag remelting, electron beam melting, investment casting, plasma spraying, and fluxless soldering.

Materials Preparation, Synthesis, Deposition, Growth or Forming

343. Investment Casting - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact F. J. Zanner, (505) 844-7073

- Investment casting is being studied with the objective of understanding fluidity as a function of alloy, mold material, mold temperature, and pouring temperature.

344. Plasma Spraying - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact M. F. Smith, (505) 846-4270

- Atmospheric and low pressure plasma spray processes are being developed to produce coatings with desirable tribological properties.
- Development of plasma sprayed diamond coatings has been initiated.

Device or Component Fabrication, Behavior or Testing

345. Laser Welding - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact J. L. Jellison, (505) 844-6397

- Both pulsed and CW laser welding is being developed for application to component closures.

- An 1800 watt CW Nd:YAG laser has been developed and quantitative measurements of fluid flow have been made.

Corrosion, Cleaning and Thin Film Technology Division, 1834

The Corrosion, Cleaning and Thin Film Technology Division 1834 conducts applied research in the areas of atmospheric, aqueous and stress corrosion. The division elucidates corrosion mechanisms using electrochemical impedance spectroscopy and acoustic sensing devices. Cleaning and contamination control processes are developed. The efficacy of these processes is studied using electron spectroscopies (AES and XPS). Thin film deposition processes are developed as a way to achieve desirable surface properties (wear resistance, corrosion resistance, electrical conductance or insulation, lubrication, etc.). Electrochemical and physical vapor deposition techniques are stressed.

Materials Preparation, Synthesis, Deposition, Growth or Forming

346. Development of Multilayer Metallizations - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Dale C. McIntyre, (505) 844-2360

- A facility has been constructed that allows multilayer metallizations to be designed using PVD techniques. These film structures are primarily designed for sealing non-metallic and metallic objects.

Materials Properties, Behavior, Characterization or Testing

347. Corrosion of Aluminum Metallization on Microelectronics - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Diane E. Peebles, (505) 845-8087

- Corrosion of aluminum metallization on VLSI is being studied as a function of Cu and Si content; fluoride ion contamination (due to HF etching processes), and metal deposition parameters.

- AES and XPS, as well as electrochemical impedance spectroscopy, are being used to elucidate the corrosion mechanisms/kinetics.

348. Characterization of Diamond Films for Tribological Applications - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Diane E. Peebles, (505) 845-8087

- Diamond films are being deposited for tribological applications using several techniques (CVD, PVD, and plasma spray).
- Non-destructive techniques for characterizing these films using electron and optical spectroscopies have been developed.
- Film degradation in reactive atmospheres, tribological properties of the films, and adhesion to selected substrates are being examined.

Device or Component Fabrication, Behavior or Testing

349. Development of Fiber-Optic Metallization for Joining - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Dale C. McIntyre, (505) 844-2360

- Multilayer metallizations are being developed as graded seals for soldering fiber optics into metallic headers.
- Physical vapor deposition techniques are being developed to reduce the stress in the metallizations on very small diameter glass fibers.
- Barrier layers are being designed to diminish long term reliability problems arising from intermetallic compound formation during and subsequent to the soldering process.

Chemistry and Ceramics Department, 1840

Department 1840 supports Sandia weapons and energy programs by selecting, developing, and characterizing ceramics, glasses and glass-ceramics. A variety of approaches are used, including gas-phase synthesis and reactions, solution preparation, as well as more traditional ceramic processing. The department promotes advanced weapons and energy concepts by providing new materials and developing new prototype components.

Interfacial Chemistry and Coating Research Division, 1841

Division 1841 is responsible for developing an understanding of the materials and processes involved in the formation of coatings and thin film structures. This work may be applicable to processes in use at Sandia, such as CVD tungsten films, as well as to new types of coatings, such as electrophoretic formation of dielectric films. The division develops CVD and aerosol techniques for preparing ceramic powders. There is a major effort in understanding the interaction of hydrogen with metals.

Electronic Ceramics Division, 1842

Division 1842 develops and determines the properties of new ceramics for electronic and optical applications in Sandia systems. Examples are PZT for nonvolatile, radiation hard semiconductor memories, high-field ZnO varistors, $KNbO_3$ for optical switches, and caprate high temperature superconductors.

Ceramics Development Division, 1845

Division 1845 is responsible for supporting laboratory programs involving glass- or ceramic-to-metal seals and other uses of glass or ceramics in moderate temperature environments. Expertise in the division includes the following areas: fracture surface analysis of brittle materials; seal design and fabrication processes; and glass and ceramic properties, i.e., strength, electrical conductivity. The division also maintains an active materials development program to formulate new glass or glass ceramics to meet particular requirements, e.g., corrosion resistance or high thermal expansion.

Inorganic Materials Chemistry Division, 1846

Division 1846 develops new processes for making ceramic powders and films using solution chemistry techniques. Understanding the structure and chemistry of sol-gel bulk and film materials is a significant part of this activity. The division also develops understanding of small particle-metal interactions that has led to new catalyst materials.

Materials Preparation, Synthesis, Deposition, Growth or Forming

350. Electrolytic and Electrophoretic Methods for Materials Processing - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Alan Hurd, (505) 846-6753

- These techniques are being used to apply organic and ceramic coatings to large irregularly-shaped objects. Applications are for composite coatings, insulators and IEMP hardeners.

351. Aerosol Production of Fine Ceramic Powders - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Alan Hurd, (505) 846-6753

- Aerosol techniques are being used to prepare fine particle, unagglomerated ceramic powders that are then further processed for electronic and structural applications.

352. Chemically Prepared Ceramic Films for Opto-electronic Applications - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact B. C. Bunker, (505) 844-8940

- Chem-prep techniques are applied to preparation of thin films of $KNbO_3$, PZT, PNZT, and other ceramics. The properties of those films are being studied and modified to enhance their performance in opto-electronic devices.

353. Development of New Glasses and Glass-Ceramics - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Peter Green, (505) 845-8929

- New formulations of glasses and glass-ceramics are being developed, primarily for sealing applications. Examples are high thermal expansion glass ceramics for sealing to stainless steel, high thermal conductivity germinate glass-ceramics, and Li-corrosion resistant glasses for battery headers.

354. Preparation of Ceramic Powders by Chemical Techniques - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact D. H Doughty, (505) 844-1933

- Chemical precipitation techniques are being developed for preparation of a wide variety of ceramic powders such as varistors, ferroelectrics, and high $T_c$ superconductors.

Materials Structure and Composition

355. Structure of Novel Glasses - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Peter Green, (505) 845-8929

- The structures of novel glasses in the phosphate tellurate and germanate systems are being studied and related to properties such as durability and thermal conductivity.

356. Structure of Sol-Gel Films - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact D. H. Doughty, (505) 844-1933

- Structures of sol-gel films suitable for optical or environmentally protective coatings are being studied by ellipsometric techniques.

Materials Properties, Behavior, Characterization or Testing

357. Molecular Beam Studies of Hydrogen in Metals - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Alan Hurd, (505) 846-6753

- Dynamics of chemical reactions on metal surfaces are studied by quantum-resolved molecular beam techniques.

358. Electronic Ceramics - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact B. C. Bunker, (505) 844-8940

- Electric properties of ceramics such as varistors, ferroelectrics and ceramic superconductors are being studied and related to composition and structure.

359. Ceramic Fracture - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Peter Green, (505) 845-8929

- Research is being conducted on ceramic fracture to understand the phenomenon better and to develop tougher ceramics.

360. Reactivity and Bonding of Glasses and Ceramics to Metals - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Peter Green, (505) 845-8929

- Reactivity of metals and ceramics are being studied to improve their bonding for hermetic seal applications.

Device or Component Fabrication, Behavior or Testing

361. Sensor Development - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact Alan Hurd, (505) 846-6753

- Environmental sensors for gases such as $H_2O$ are being developed using porous ceramic films grown by electrolytic techniques.

362. SAW Development - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact D. H. Doughty, (505) 844-1933

- Surface acoustic wave devices are being developed as sensitive and selective detectors are adsorbed species in gas and liquid environments.

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

363. Powder Metallurgy - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact J. E. Smugeresky, (294) 422-2910

- Inert gas atomization and chemical processes are being used to advance development of the powder metallurgy and rapid solidification processing of a variety of pure metals and alloy systems. Advanced techniques are being developed and applied to powder characterization.

364. Advanced Electrodeposition Studies - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts R. E. Stoltz, (415) 294-2162, H. R. Johnson, (415) 294-2822 and W. D. Bonivert, (415) 294-2987.

- Engineering applications, electroanalytical development, and fundamental investigations are being pursued in the area of electrodeposition and electroforming. Special attention is given to reductions in use of hazardous materials and to waste minimization.

365. Metal Forming - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact D. A. Hughes, (415) 294-2686

- Inelastic deformation and failure are examined through crystal plasticity modeling and experimentation. Results are used to help interpret finite element metal forming simulations and guide the development of phenomenological constitutive relations for large strain deformation.

366. Advanced Foam Materials - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts D. L. Lindner, (415) 294-3306, W. R. Even, (415) 294-3217 and C. B. Frost, (415) 294-2048

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

367. Tritium Getter Technology - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; Sandia Contacts D. L. Lindner, (415) 294-3306 and T. Shepodd, (415) 294-2791

- We have demonstrated a system that is capable of gettering large amounts of tritium gas even in the presence of contained amounts of oxygen and water without releasing radioactive species as it ages.

368. Plasma Processing - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contact W. L. Hsu, (415) 294-2379

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

Materials Properties, Behavior, Characterization or Testing

369. Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts S. L. Robinson, (415) 294-2209, S. H. Goods, (415) 294-3274 and N. R. Moody, (415) 294-2622

- Experimental and theoretical studies are underway to determine the effects of tritium and decay helium on mechanical properties and crack growth susceptibility in fcc alloys.

370. Joining Science and Technology - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts J. A. Brooks, (415) 294-2051, K. W. Mahin, (415) 294-3582 and M. C. Callabressi, (415) 294-2064

- This program is developing a science-based methodology for improving the fundamental understanding of the behavior of welded structures and modeling of the complex fusion weld process. Advanced joining techniques using solid state welding, and adhesives are being developed for advanced structural materials.

371. Composites: Characterization and Joining - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts D. L. Lindner, (415) 294-3306 and J. R. Spingarn, (415) 294-2719

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

372. Compatibility, Corrosion, and Cleaning of Materials - DOE Contact, C. B. Hilland, (301) 353-3687; Sandia Contacts H. R. Johnson, (415) 294-2822, R. E. Stoltz, (415) 294-2162, J. M. Hruby, (415) 294-2596 and D. K. Ottesen, (415) 294-2787

- We have developed special techniques using FTIR that allow interior surface of small diameter tubes or external surfaces of wire are examined for corrosion and efficacy of improved cleaning techniques.

373. Helium in Metal Tritides - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts W. A. Swansiger, FTS 234-2496, S. E. Guthrie, FTS 234-2360 and D. F. Cowgill, (505) 844-7480

- Helium evolution in metal tritides is being studied by NMR, gas sampling and dilatometry techniques.

Instrumentation and Facilities

374. Tritium Facility Materials Characterization and Testing - DOE Contact C. B. Hilland, (301) 353-3687; Sandia Contacts S. H. Goods, (415) 294-3274 and S. L. Robinson, (415) 294-2209

- New experimental capabilities in surface analysis, fractography, and thermomechanical history are improving both the characterization of tritium-induced degradation of material properties, and the development of predictive abilities.

375. New Analytical Techniques - DOE Contact C. B. Hilland, (301) 353-3687/ FTS 233-3687; Sandia Contacts D. L. Lindner, (415) 294-3306, M. C. Nichols, (415) 294-2906 and B. E. Mills, (415) 294-3230

- We have developed a system for X-ray microtomography that can be used for spatial elemental analysis for materials and structures.

376. New High Resolution Electron Microscopy Facility - DOE Contact C. B. Hilland; (301) 353-3687; Sandia Contacts G. J. Thomas, (415) 294-3224 and M. J. Mills, (415) 294-3018

- A new high resolution transmission electron microscope laboratory is now operational. It will be utilized to investigate: (a) metal-metal interfaces such as grain boundaries; (b) defect structures in undeformed and deformed metals and alloys; (c) helium-induced defect evolution in metal tritides; and (d) semiconductor-oxide interfaces.

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

377. Inorganic Aerogels - DOE Contact C. B. Hilland, (301) 353-3687/FTS 2333687; LLNL Contact L. W. Hrubesh, (415) 423-1691/FTS 543-1691

- The objective of this project is to develop the chemistry and procedures for processing monolithic pieces of micro-porous, inorganic aerogel materials and to extend the range of bulk densities over which such materials can be directly made.

378. Photoactivated Catalysis on Aerogels - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact C. A. Colmenares, (415) 422-6352/FTS 532-6352

- We have demonstrated that $SiO_2$ aerogels doped with uranyl ions are catalytically active for the production hydrocarbons from simple gas mixtures (i.e., Co + $H_2$, $H_2+C_2H_4$, and $H_2$ + $C_2H_6$) using sunlight as the energy source. We are currently investigating other dopants (i.e., $Ce^{IV}$, $Eu^{IV}$, $Fe^{+3}$, and others) and the basic energy transfer mechanism using surface-sensitive and optical spectroscopies.

379. Organic Aerogels - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact R. W. Pekala, (415) 422-0152

- This project examines the synthesis of aerogels from organic precursors using sol-gel chemistry.

380. Polymer Materials Development and Coating - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact S. A. Letts, (415) 423-2681/FTS 543-2681

- Low density, porous, polymer foams are being developed to hold liquid DT fuel for direct-drive laser fusion targets. Ultra smooth, uniform plasma polymer coatings are being developed as ablator layers for direct-drive laser targets.

381. Atomic Engineering - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact Troy W. Barbee, Jr., (415) 423-7796/FTS 543-7796

- Physical vapor deposition techniques are being used to synthesize ordered compounds by a sequential atomic layer technique. Control of the process has led to free standing foils with extraordinary mechanical properties.

Materials Structure and Composition

382. Theory of the Structure and Dynamics of Molecular Fluids - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact D. F. Calef, (415) 422-7797/FTS 532-7797

- Develop improved theoretical models for the thermodynamic and kinetic behavior of molecular fluids, especially under the conditions of extreme pressure and temperature found in detonations.

383. Plutonium Pyrochemical Research - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; LLNL Contact M. Coops, (415) 422-8076

- Proof of principle was demonstrated for a lithium-based process to reduce Pu oxide to metal with little waste or residue.

384. Electronic Structure in Superconducting Oxides - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; LLNL Contact M. J. Fluss, (415) 423-6665/FTS 543-6665

- We have put into place a multidisciplinary program involving the chemistry, physics, and technology of high-temperature superconductors with the goal of deducing the mechanism underlying their properties.

385. Electronic Structure Study of the Thermodynamic and Mechanical Properties of Al-Li Alloys - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; LLNL Contact A. Gonis, (415) 423-5836/FTS 543-5836

- The objective of this research is to develop first-principles, charge self-consistent methods for the determination of the electronic structure of surfaces and grain boundaries.

Materials Properties, Behavior, Characterization or Testing

386. Nuclear Spin Polarization - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; 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.

387. Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures - DOE Contact C. B. Hilland, (301) 353-3687; FTS 2333687; LLNL Contact Jon L. Maienschein, (415) 423-1816/FTS 543-1816

- Measuring tritium permeation through resistant materials at 10-170°C, using a very sensitive method developed in this laboratory, to enhance our understanding of the permeation process at low temperatures.

388. Pretransformation Behavior in Alloys - DOE Contact A. Dragoo, (202) 586-5276; 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.

389. The Structure Property Link in Sub-Nanometer Materials - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact A. F. Jankowski, (415) 523-2519/FTS 543-2519

- The motivation for this study was to determine the cause for differences measures in the X-ray reflectivities between W/C and newly developed W/$B_4$C multilayer X-ray mirrors.

390. Synchrotron Radiation-Based Materials Science - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact J. Wong, (415) 423-6385/FTS 543-6385

- The objective of this research is the use of synchrotron radiation to understand the role of structure (atomic and electronic) in determining the physico-chemical properties of materials and their processing.

391. Structural Transformation and Precursor Phenomena - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact P. E. A. Turchi, (415) 422-9925/FTS 532-9925

- The main objective is to study, both theoretically and experimentally, the occurrence and stability of a class of advanced materials known as tetrahedrally close packed structures with special emphasis on precursor phenomena.

392. Underwater Explosive Energetics - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. C. Tao, (415) 423-0499/FTS 543-0499

- The rapid combustion of reactive metals in water is examined both experimentally and by modeling.

393. Composite Explosive Energetics - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. C. Tao, (415) 423-0499/FTS 543-0499

- The role of metal additives in bicomponent composite explosives is studied with metal acceleration techniques and reactive flow modeling.

394. Low Vulnerability Explosives - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact C. Pruneda, (415) 422-0460/FTS 532-0460

- The optimization of quality and insensitivity is extended to larger diameter systems by adjustments to the polymer binder and formulation composition.

395. Fundamentals of Explosive Vulnerability - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. C. Tao, (415) 423-0499/FTS 543-0499

- Correlation of explosive response with material properties of the explosive such as modulus, binder energy, explosive particle size.

396. Very High Energy Density Materials - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact R. L. Simpson, (415) 423-0379/FTS 543-0379

- The sensitivity and performance properties of the explosive Cl-20 have been examined in both the alpha and epsilon phases.

397. Use of Finite Element Analysis to Understand Delayed Failure in Silver Interlayer Welds - DOE Contact C. B. Hilland, (301) 353-5687; LLNL Contact G. A. Henshall, (415) 422-3290/FTS 532-3290

- Theory and experiments were used to describe the performance of interlayer diffusion bonds under elastic and plastic loading.

398. Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. H. Gourdin, (415) 422-8673/ FTS 532-8673

- The results of electromagnetically launched expanding-ring experiments and conventional compression tests with oxygen free electronic (OFE) copper of grain size 10 to 200 $\mu$m are reported and analyzed in terms of the mechanical threshold stress (MTS) model.

- Overall the model provides an excellent description of the material behavior over a wide range of grain size, strain rate and temperature.

399. Theoretical and Experimental Studies of Solid Combustion Reactions - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact J. B. Holt, (415) 422-8003/FTS 532-8003

- The objectives of this work were to develop a mathematical model for condensed phase combustion involving a sequential reaction mechanism and to determine kinetic constants for a model reaction such as Ti and C.

400. Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; LLNL Contact J. S. Huang, (415) 422-5645

- This investigation characterizes the mechanical behaviors of refractory metals and alloys in liquid actinides. The emphasis is on the study of micromechanisms of fracture and of the relations between phase diagrams and micromechanisms of fracture.

401. Oxidation and Liquid Metal Resistant Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact O. H. Krikorian, (415) 423-4655/FTS 543-4655

- Aluminide and silicide coatings have been developed to provide excellent oxidation resistance for refractory alloys

402. Development of Ultrafine Microstructures Through Rapid Solidification Rate Processing - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact J. W. Elmer, (415) 423-4655/FTS 543-4655

- Rapid solidification has produced ultrafine particles in a dilute hyper-eutecoid alloy.

403. Failure Characterization of Composite Materials - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact Scott E. Groves, (415) 422-1331/FTS 532-1331

- The primary objective of this research is to characterize the three-dimensional failure response of continuous fiber graphite epoxy composite materials.

404. Modeling Superplastic Materials - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact Donald Lesuer, (415) 422-9633/FTS 532-9633

- We are developing a model that describes the influence of structural change (primarily grain growth and cavitation) on the deformation and failure of superplastic materials.

405. Creep Model for Fiber Reinforced Epoxy-Resin Composites - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact William W. Feng, (415) 422-8701/ FTS 532-8701

- A mathematical model of creep in a fiber reinforced epoxy-resin laminated composite has been developed.

406. Superplastic Flow of Ceramics and Intermetallics - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact E. N. C. Dalder, (415) 422-7270/FTS 532-7270

- We are studying the influence of temperature and strain rate for superplastic behavior of a silicon nitride ceramic and a titanium aluminide intermetallic as functions of starting microstructure.

407. Structural Joints for Composite Materials - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact Frank Magness, (415) 423-1324/FTS 533-1324

- We have assessed the state-of-the-art in composites joining and evaluated laboratory capability for modeling specific design requirements in composite joints.

408. Interfaces, Adhesion and Bonding - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact Wayne E. King, (415) 423-6547/FTS 543-6547

- Investigation of the influence of impurities, flaws, and inclusions on adhesion and bonding at internal interfaces. The initial phase is characterization of the structure and properties of pure interfaces as a baseline for future research.

Device or Component Fabrication, Behavior or Testing

409. IC Protective Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact M. O. Riley, (415) 422-6865/FTS 532-3045

- The goal of this work is the development of protective coatings to safeguard microelectronic chips.

410. Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. C. Tao, (415) 423-0499/FTS 543-0499

- The objectives of this research are to characterize non-des[illegible]ely the type and distribution [illegible]rostructural defects in high explosive singl[illegible]s and composite formulation, and to examine their respective influences on H[illegible]t generation and propagation.

411. Optical Diagnostics of High Explosives Reaction Chemistry - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact R. L. Simpson, (415) 423-3258/FTS 543-3258

- The objectives of this research are to develop time resolved techniques to study the molecular and microscopic behavior of the reaction zone of detonating and deflagrating energetic materials. Special emphasis is placed on pulsed laser probes designed to study the chemical kinetics of reactions under these conditions.

Instrumentation and Facilities

412. Scanning Tunneling Microscopy - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. Siekhaus, (415) 422-6884/FTS 532-6884

- The technical objectives of this program are to develop STM's capable of performing (with atomic resolution) structural analysis and spectroscopic analysis in fluids (air, water, oil) and in ultrahigh vacuum (UHV).

413. Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact W. Siekhaus, (415) 422-6884/FTS 532-6884

- Scanning tunneling microscopy, in conjunction with the atomic force microscope, are now used: (1) to detect and characterize submicron defects on optical components which may be conductors or insulators and to determine their effect on laser surface damage threshold, (2) to study the growth morphology of optical and X-ray multilayers, (3) to study gas-surface reaction rates as low as one Angstrom per day.

414. Tritium Facility Upgrade - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact J. H. Richardson, (415) 423-1770/FTS 543-1770

- Consists of three line items: (1) a new 5,700 square foot office addition along with the modification of 2,000 square feet of the existing facility, (2) a Vacuum Effluent and Recovery System (VERS) designed to recover over 90 percent of the existing routine stack emissions, (3) a Secondarily Contained Tritium System (SCOTS) which replaces the existing low and high pressure systems with a modern totally secondarily contained system.

415. Decontamination and Waste Treatment Facility (DWTF) - DOE Contact C. B. Hilland, (301) 353-3687; LLNL Contact R. Quong, (415) 422-7093/FTS 532-7093

- The proposed Decontamination and Waste Treatment Facility (DWTF) will provide complete radioactive, mixed, and hazardous waste treatment capability of laboratory generated wastes.

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

416. Actinide Processing Development - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. F. Stevens, (505) 667-4414/FTS 843-4414

- Development of new processing technologies for plutonium, including casting, thermomechanical working, sputtering, and stability studies.

- Measurements of resistivity, thermal expansion, magnetic susceptibility and formability to evaluate fabrication processes and alloy stability.

417. Plutonium Oxide Reduction - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact K. Axler, (505) 667-4045/FTS 843-4045

- Determination of thermodynamics of interactions used in direct-oxide reduction of plutonium.

418. Ion-Beam Implantation - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Scott, (505) 667-7757/FTS 843-7757

- Exploration of ion implantation for surface modification.

- Goals of improved surface hardness and corrosion resistance.

419. Electroplating Low Atomic Number Materials - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact T. Mayer, (505) 667-1146/FTS 843-1146

- Investigation of electroplating low atomic number metals (aluminum and beryllium) by using non-aqueous plating baths.

420. Liquid Crystal Polymer Development - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact R. Liepens, (505) 667-2656/FTS 843-2656

- Synthesis of a liquid crystal polymer with strength in three dimensions.

421. Low-Density, Microcellular Plastic Foams - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact J. Williams, (505) 667-7881/FTS 843-7881

- Manufacture of microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc by a nonconventional foaming process.

422. Target Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Scott, (505) 667-7557/FTS 843-7557

- Development of single and multilayer metallic and nonmetallic thin film coatings, smooth and uniform in thickness.

423. Physical Vapor Deposition and Surface Analysis - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Scott, (505) 667-7557/FTS 843-7557

- Physical vapor deposition and sputtering to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers.

424. Chemical Vapor Deposition (CVD) Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contacts J. R. Laia and M. Tekuia, (505) 667-3239/ FTS 843-3239

- Development of CVD thin film and bulk coatings by a variety of techniques including conventional flow-by, fluid-bed, plasma-assisted, MOCVD, and chemical vapor infiltration (CVI) in support of DOE, DOD, and other Federal agency programs.

- Synthesis/application of new CVD organometallic precursors for low temperature ($<300^\circ C$) deposition.

- *In-situ* diagnostics of CVD reactors/processes using various spectroscopies to feed back data for process control (intelligent processing).

- Modeling activities in support of CVD coating systems—reactor systems, chemical systems, and fluid dynamics.

- Laser-assisted CVD and laser material interactions.

425. Polymers and Adhesives - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact D. A. Hemphill, (505) 667-8335/FTS 843-8335

    - Development of fabrication processes and evaluation and testing of commercial and special plastic and composite materials for weapons programs.

    - Development of highly filled polymers, composite structural and spring components, cushioning materials, high-explosive compatible adhesives, potting materials, and castable loaded thermoplastics.

    - Goal is improving weapon efficiency and economy.

426. Tritiated Materials - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact D. H. W. Carstens, (505) 667-5849/FTS 843-5849

    - Advanced R&D on low-Z, tritiated materials with the emphasis on Li(D,T) (salt) and other metal tritides.

    - Studies of new methods for preparing, fabricating, and containing such compounds, and for measurement of properties.

427. Salt Fabrication - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact D. H. W. Carstens, (505) 667-5849/FTS 843-5849

    - Development and evaluation of fabrication processes for lithium tritide deuteride.

    - Use of hot pressing and machining to improve part shape versatility, density, and surface quality.

    - Conduct of component integrity studies involving radiation induced growth and outgassing.

428. Slip Casting of Ceramics - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact G. F. Hurley, (505) 667-9498/FTS 843-9498

- Slip casting of many ceramics including alumina, magnesia, and thoria.

- Use of colloidal chemistry and powder characterization theory along with materials engineering.

429. Glass and Ceramic Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact R. E. Honnell, (505) 667-5432

- Fabrication of ceramic-metal seals, insulating coatings, and metallurgy.

430. Cold Pressing, Cold Isostatic Pressing and Sintering - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact G. F. Hurley, (505) 667-9498/FTS 843-9498

- Use of cold pressing and cold isostatic pressing to consolidate ceramic and metal powders in support of laboratory programs.

431. Plasma-Flame Spraying Technology - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Fabrication of free-standing shapes, and metallic and ceramic coatings by plasma spraying.

432. Rapid Solidification Technology - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact H. Casey, (505) 667-4365/FTS 843-4365

- Development of RSR technologies such as melt spinning, splat cooling, and rapid solidification plasma spraying.

- Alloy development, microstructural analysis, properties testing, process development, modeling.

433. Microwave Sintering/Processing - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact J. D. Katz, (505) 667-1424/FTS 843-1424

- Investigating techniques of bonding and sintering ceramics such as $Al_20_3$, $B_4C$ and $TiB_2$.

- Use of 2.45 GHz microwaves which couple directly to the area in which the heat is needed.

- Investigation of the control of the heating and its effect on microstructure.

434. Predictions of Super Strong Polymers - DOE Contact Iran Thomas, (301) 353-3427/ FTS 233-3427; LANL Contact F. Dowell, (505) 667-8765/FTS 843-8765

- First-principles mathematical models have been developed to predict (with the aid of computer-based modeling) new molecular structures most likely to form super strong polymers. Other properties are being predicted.

- Candidate molecules are being chemically synthesized and will be experimentally characterized.

435. Synthesis of Ceramic Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LANL C. P. Scherer, (505) 665-3202

- Synthesis of ceramic coatings via sol gel techniques.

436. Laser Surface Treatment of Materials - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Nastase, (505) 667-7007/FTS 843-7007

- Laser treatment of metallic surfaces to modify properties such as coefficient of friction and corrosion resistance.

Materials Structure or Composition

437. Actinide Surface Properties - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. F. Stevens, (505) 667-2556/FTS 843-2556

- Characterization of actinide metal, alloy and compound surfaces using the techniques of X-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy.

- Studies of surface reactions, chemisorption, attack by hydrogen, nature of associated catalytic processes.

438. Neutron Diffraction of Pu, Pu Alloys and Other Actinides - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact A. C. Lawson, (505) 667-8844/FTS 843-8844

- Neutron diffraction studies of plutonium and its alloys conducted at the Manual Lugan, Jr., Neutron Scattering Center (Los Alamos) and the Intense Pulsed Neutron Source (Argonne).

- Time-of-flight technique used to measure diffraction at cryogenic and elevated temperatures.

439. Surface, Material and Analytical Studies - DOE Contact C. B. Hilland, (301) 353-3687/ FTS 233-3912; LANL Contact W. C. Danen, (505) 667-4686

- Studies of surface and interfacial structures and properties, explosive dynamics, and laser based isotopic analysis.

- Use of techniques such as Low Energy Electron Diffraction (LEED), Auger and Loss Spectroscopies, Ion-Scattering Spectroscopy (ISS), Ultraviolet Photoelectron Spectroscopy (UPS), Synchrotron Radiation, and MeV-ion-beam scattering.

- Synthesis and characterization of metastable multilayerd high-energy-density composite materials.

Materials Properties, Behavior, Characterization or Testing

440. Mechanical Properties of Plutonium and Its Alloys - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Stevens, (505) 667-4414/FTS 843-4414

- Study relationship of mechanical properties of Pu and Pu alloys to their microstructures.

- Use of optical and electron microscopy, X-ray, electron, and neutron diffraction.

441. Phase Transformations in Pu and Pu Alloys - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Stevens, (505) 667-4414/FTS 843-4414

- Investigation of mechanisms, crystallography, and kinetics of transformations in plutonium and alloys using pressure and temperature dilatometry, optical metallography, and X-ray diffraction.

442. Plutonium Shock Deformation - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. J. Reisfeld, (505) 667-8485/FTS 843-8485

- Plutonium alloys subjected to shock deformation, recovered and examined to determine effects of shock on microstructures and mechanical properties.

443. Non-Destructive Evaluation - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Mathieson, (505) 667-6404/FTS 843-6404

- Development of nondestructive evaluation technology that produces quantitative estimates of material properties.

- Flash radiography, cine radiography, real time radiography, ultrasonic in-process probing, and tomographic techniques to enhance radiography. Image enhancement of output results from all techniques.

444. Powder Characterization - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact G. J. Vogt, (505) 667-5813

- Characterization of particle size, surface area, morphology, pore size and zeta potential.

- Powders of thoria, silicon nitride, magnesia, alumina, tungsten, tungsten carbide, and copper.

445. Shock Deformation in Actinide Materials - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact M. Stevens, (505) 667-4414/FTS 843-4414

- Characterization of shock effects in uranium, plutonium and plutonium alloys through use of soft recovery techniques.

446. Dynamic Mechanical Properties of Weapons Materials - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact G. Gray, (505) 667-5452/FTS 843-5452

- Dynamic stress-strain and fracture behavior of non-nuclear materials for nuclear weapons.

447. Dynamic Testing of Materials for Hyper-Velocity Projectiles - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact G. T. Gray, III, (505) 667-5452/ FTS 843-5452

- Microstructural characterization of dynamically deformed and spalled high density materials.

- Dynamic and quasi-static mechanical testing.

448. Mechanical Properties - DOE Contact R. J. Gottschall, (301) 353-3428/FTS 233-3428; LANL Contact M. G. Stout, (505) 667-4665/FTS 843-4665

- Multiaxial testing of metal and alloys.

- Prediction of texture development and its effects.

Device or Component Fabrication, Behavior or Testing

449. Radiochemistry Detector Coatings - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact G. Reeves, (505) 667-4290/FTS 843-4290

- Physical vapor deposition of coatings for radiochemical detectors.

450. Target Fabrication - DOE Contact C. B. Hilland, (301) 353-3687/FTS 233-3687; LANL Contact L. Foreman, (505) 667-1846/FTS 843-1846; KMS Fusion, Inc., Contact Timothy Henderson, (313) 769-8500, ext. 302; LLNL Contact W. Hatcher, (415) 422-1100

- Hydrocarbon polymer applied by plasma polymerization to glass microspheres.

- Micromachining, plasma etching, plasma polymerization, laser ablation.

- Targets filled with deuterium/tritium gas.

451. Filament Winder - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact E. Eaton, (505) 667-5261/FTS 843-5261

- Four-axis computer-programmed winding machine.
- Winding envelopes to 4 ft. diameter, 10 ft. long.
- Winds helixes, cones, spheres, closed-end vessels of glass, kevlar, carbon, tungsten, and alumina fibers.

452. Polymeric Laser Rods - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact R. Hermes, (505) 667-6862/FTS 843-6862

- Development of polymeric-host dye-laser rods.
- *In situ* polymerization of dye/monomer mixture.
- Inexpensive "disposable" laser rods.

453. High Energy Density Welding in Hazardous Environments - DOE Contact C. B. Hilland, (301) 353-3687; LANL Contact R. A. Patterson, (505) 667-4365/ FTS 843-4365

- Utilization of high power Nd/YAG lasers with fiber optic beam delivery for welding in hazardous environments has been demonstrated.

# OFFICE OF FOSSIL ENERGY

| | FY 1990 |
|---|---|
| Office of Fossil Energy - Grand Total | $7,031,000 |
| Office of Technical Coordination | $7,031,000 |
| Fossil Energy AR&TD Materials Program | $7,031,000 |
| Materials Preparation, Synthesis, Deposition, Growth or Forming | $2,187,000 |
| Fundamental Study of Aluminizing and Chromizing Processes | 99,000 |
| Procurement of Advanced Austenitic and Aluminide Alloys | 49,000 |
| Iron Aluminide Processing | 34,000 |
| Development of Iron Aluminides | 382,000 |
| Welding Processing | 34,000 |
| Development and Evaluation of Advanced Austenitic Alloys | 257,000 |
| Evaluation of the Fabricability of Advanced Austenitic Alloys | 26,000 |
| The Influence of Processing on Microstructure and Mechanical Properties of Aluminides | 173,000 |
| Evaluation of the Fabricability of Iron Aluminides | 25,000 |
| Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres | 106,000 |
| Vapor-Liquid-Solid SiC Whisker Process Development | 99,000 |
| Ceramic Composite Processing | 35,000 |
| Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition | 188,000 |
| Characterization of Fiber-CVD Matrix Interfacial Bonds | 138,000 |
| Microwave Sintering of Ceramics | 197,000 |
| Development of Advanced Fiber Reinforced Ceramics | 148,000 |
| Modeling of Fibrous Preforms for CVD Infiltration | 49,000 |
| Electroslag Casting Technology Transfer | 148,000 |
| Materials Structure and Composition | $ 279,000 |
| Analytical Characterization of Coal Surfaces and Interfaces | 279,000 |

## OFFICE OF FOSSIL ENERGY (Continued)

| | FY 1990 |
|---|---|
| Materials Properties, Behavior, Characterization or Testing | $2,713,000 |
| Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry | 82,000 |
| Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys | 138,000 |
| Investigation of the Weldability of Ductile Aluminides | 74,000 |
| Aqueous Corrosion of Iron Aluminides | 49,000 |
| Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings | 0 |
| Joining Techniques for Advanced Austenitic Alloys | 148,000 |
| Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments | 316,000 |
| Environmental Effects on Iron Aluminides | 192,000 |
| Secondary-Ion Mass Spectrometry Study of Scales on Iron Aluminides | 15,000 |
| Investigation of Moisture-Induced Embrittlement of Iron Aluminides | 59,000 |
| The Effect of Alloying Constituents and Control of the Growth of Protective Oxide Scales | 0 |
| Effect of Reactive Element Additions on the Protectiveness of Oxide Scales Formed in Sulfur-Containing Atmospheres | 0 |
| Effects of Several Variables on the Growth and Breakdown of Protective Alumina or Chromia Scales in Mixed-Gas Environments | 0 |
| Molten Salt-Induced Corrosion of Iron Aluminides | 0 |
| A Study of Erosive Particle Rebound Parameters | 0 |
| Studies of Materials Erosion in Coal Conversion and Utilization Systems | 247,000 |
| Responses of Metallic and Oxide Surfaces to Deformation | |
| Study of Particle Rebound Characteristics and Material | 192,000 |
| Erosion at High Temperatures | 109,000 |
| Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics | 311,000 |
| Joining of Silicon Carbide Reinforced Ceramics | 173,000 |

## OFFICE OF FOSSIL ENERGY (Continued)

| | FY 1990 |
|---|---|
| Materials Properties, Behavior, Characterization or Testing (continued) | |
| Nondestructive Evaluation of Advanced Ceramic Composite Materials | 172,000 |
| Structural Reliability and Damage Tolerance of Ceramic Composites | 148,000 |
| Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites | 91,000 |
| Ceramic Catalyst Materials: Hydrous Metal Oxide Ion Exchange Supports for Direct Coal Liquefaction | 197,000 |
| Device or Component Fabrication, Behavior or Testing | $1,338,000 |
| *Materials and Components in Fossil Energy Applications* (Newsletter) | 114,000 |
| Mechanisms of Galling and Abrasive Wear | 74,000 |
| Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition | 0 |
| Development of Ceramic Membranes for Gas Separation | 327,000 |
| Investigation of the Mechanical Properties and Performance of Ceramic Composite Components | 0 |
| Material Data Base Development for Refractories | 0 |
| Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes | 296,000 |
| Gas Separations Using Inorganic Membranes | 197,000 |
| Ceramic Fiber-Ceramic Matrix Hot-Gas Filters | 197,000 |
| Identification of Materials for Hot-Gas Filter Tubesheets | 133,000 |
| Instrumentation and Facilities | $ 514,000 |
| Management of the Fossil Energy AR&TD Materials Program | 396,000 |
| Materials Specialist Assignment | 69,000 |
| Coal Conversion and Utilization Plant Support Services | 49,000 |
| Assessment of Fossil Energy Materials Research Needs | 0 |

## OFFICE OF FOSSIL ENERGY (Continued)

| | | FY 1990 |
|---|---|---|
| Office of Coal Technology | $ | 0 |
| Division of Clean Coal Technology | $ | 0 |
| Instrumentation and Facilities | $ | 0 |
| Materials Technical Support for the Clean Coal Program | | 0 |

# OFFICE OF FOSSIL ENERGY

The mission of the Fossil Energy Program is to develop technologies that will increase domestic production of oil and gas or that will permit the Nation to shift from oil or gas to more abundant coal. Specifically, the Fossil Energy role is to develop technologies to support the following objectives:

- Provide a capability to convert coal to liquid and gaseous fuels;
- Increase domestic production of coal, oil, and gas;
- Ensure that current and new facilities that burn coal can do so in an economically viable and environmentally acceptable manner; and
- Allow more efficient and more economically attractive utilization of fossil energy resources.

The Fossil Energy activity includes fourteen major programs, which are grouped under seven program offices. One of these seven is the Advanced Research and Technology Development Program of the Office of Technical Coordination, which is the central point of contact for inquiries from universities concerning the Fossil Energy program.

Project execution and technical monitoring are administered in five energy technology centers and selected national laboratories.

## Office of Technical Coordination

### Fossil Energy AR&TD Materials Program

The objectives of the Advanced Research and Technology Development program are to assess and identify long-range advanced research needs in coal processing, fossil fuels utilization and extraction, materials, components, and instrumentation; to provide oversight of ongoing advanced research in fossil energy so as to ensure balance and proper priorities; to initiate and fund projects involving new, exploratory concepts or goal-oriented basic research; to manage the Materials Research and University Coal Research programs; and to provide policies for, and overview of, Fossil Energy-supported university activities. The Advanced Research and Technology Development program also is designed to provide an effective communications channel between the Fossil Energy program and academic institutions; to encourage these institutions to become involved in programs related to the DOE Fossil Energy mission; and to manage programs concerned with providing an adequate technical base for development of commercial construction materials and instrumentation for Fossil Energy pilot plants and demonstration plants.

The program supports workshops to identify research needs in all fossil energy technologies and manages selected training programs for faculty and students at Energy Technology Centers.

Materials Preparation, Synthesis, Deposition, Growth or Forming

454. Fundamental Study of Aluminizing and Chromizing Processes - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Ohio State University Contact R. A. Rapp, (614) 292-6178

- The purpose of this work is to conduct a study of aluminizing and chromizing of iron-base alloys which will lead to a fundamental understanding of these processes.

455. Procurement of Advanced Austenitic and Aluminide Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- This task provides funds for the procurement of alloys necessary for alloy development and evaluation activities on the Fossil Energy AR&TD Materials Program.

456. Iron Aluminide Processing - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- This task provides funds for the procurement of major equipment items necessary for iron aluminide development activities on the Fossil Energy AR&TD Materials Program.

457. Development of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/ FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact C. G. McKamey, (615) 574-6917/FTS 624-6917

- The objective of this project is to develop low-cost and low-density intermetallic alloys based on $Fe_3Al$ with an optimum combination of strength, ductility, and corrosion resistance for use as components in advanced fossil energy conversion systems.

458. Welding Processing - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- This task provides funds for the procurement of major equipment items necessary for welding activities associated with alloy development projects on the Fossil Energy AR&TD Materials Program.

459. Development and Evaluation of Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Oak Ridge National Laboratory Contact R. W. Swindeman, (615) 574-5108/FTS 624-5108

- The purpose of this project is to evaluate austenitic alloys for improved performance in high-temperature components in advanced heat recovery and hot-gas cleanup systems.

460. Evaluation of the Fabricability of Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Babcock & Wilcox Contact M. J. Topolski, (216) 829-7301

- The purpose of this work is to evaluate the fabricability, weldability, and surface treatments of advanced austenitic tubing for superheater applications.

461. The Influence of Processing on Microstructure and Mechanical Properties of Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Idaho National Engineering Laboratory Contact R. N. Wright, FTS 583-6127

- The purpose of this project is to develop techniques for processing intermetallic compounds to improve their room-temperature ductility and elevated-temperature mechanical properties.

462. Evaluation of the Fabricability of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Pittsburgh Contact H. D. Brody, (412) 624-9724

- The purpose of this project is to evaluate and improve the casting characteristics of iron aluminides.

463. Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Westinghouse Hanford Company Contact R. N. Johnson, (509) 376-3582

- The objective of this task is to investigate a novel coating technology, electrospark deposition, for the production of cost-effective metallurgical coatings to protect materials from both erosion and corrosion in sulfidizing environments typical of fossil energy systems.

464. Vapor-Liquid-Solid SiC Whisker Process Development - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Los Alamos National Laboratory Contact J. D. Katz, (505) 665-1424/FTS 855-1424

- The purpose of this project is to provide assistance in transferring the laboratory-scale Vapor-Liquid-Solid (VLS) SiC whisker growth process to an industrial organization for engineering-scale development.

465. Ceramic Composite Processing - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6509 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- This task provides funds for the procurement of major equipment items necessary for ceramic composite development and characterization activities on the Fossil Energy AR&TD Materials Program.

466. Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition (CVID) -DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contacts D. P. Stinton, (615) 574-4556/FTS 624-4556

- The purpose of this task is to develop a process for the fabrication of fiber-reinforced ceramic composites having high fracture toughness and high strength.

467. Characterization of Fiber-CVD Matrix Interfacial Bonds - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. A. Lowden, (615) 574-7714/FTS 624-7714

- The purpose of this task is to examine fiber-matrix interfaces and optimize the mechanical behavior of continuous fiber-reinforced ceramic composites fabricated utilizing a forced-flow, thermal-gradient chemical vapor infiltration technique.

468. Microwave Sintering of Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contacts M. A. Janney and H. D. Kimrey, (615) 574-4281/FTS 624-4281

- The purpose of this activity is to explore the feasibility of using microwave heating as a means of fabricating electrode, electrolyte, and interconnect materials having improved electrical properties for solid oxide fuel cells.

469. Development of Advanced Fiber Reinforced Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Georgia Institute of Technology Contact T. L. Starr, (404) 894-3678

- The purpose of this research effort is to conduct a theoretical and experimental program to identify new compositions and processing methods to improve the physical and mechanical properties of selected fiber reinforced ceramics.

470. Modeling of Fibrous Preforms for CVD Infiltration - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Georgia Institute of Technology Contact T. L. Starr, (404) 894-3678

- The purpose of this project is to conduct a theoretical and experimental program to develop an analytical model for the fabrication and infiltration of fibrous preforms.

471. Electroslag Casting Technology Transfer - DOE Contacts V. Kothari, FTS 923-4505 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact V. K. Sikka, (615) 574-5112/FTS 624-5112

- The purpose of this project is to transfer the electroslag casting technology foro iron aluminides to industry.

Materials Structure and Composition

472. Analytical Characterization of Coal Surfaces and Interfaces - DOE Contacts J. D. Hickerson, FTS 723-5721 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact V. J. Tennery, (615) 574-5124/FTS 624-5124

- The objective of this task is to provide analytical characterization of coal surfaces and interfaces between coal and various included minerals for the purpose of assisting the Pittsburgh Energy Technology Center in its research on coal characterization and cleaning.

Materials Properties, Behavior, Characterization or Testing

473. Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Tennessee Center for Research and Development Contact A. H. von der Esch, (615) 675-9505

- The purpose of this activity is to develop user-friendly and intelligent computer-based software for the prediction of thermomechanical behavior of refractory lining systems.

474. Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Cornell University Contact Che-Yu Li, (607) 256-4349

- The purpose of this project is to rank the strengths and metallurgical stabilities of advanced austenitic alloys at temperatures ranging from 650° to $760^0$°C.

475. Investigation of the Weldability of Ductile Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Colorado School of Mines Contact G. R. Edwards, (303) 273-3773

- The purpose of this project is to study the weldability of iron aluminides.

476. Aqueous Corrosion of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Tennessee Contact R. A. Buchanan, (615) 974-4858

- The objective of this project is to investigate the aqueous corrosion of iron aluminides based on $Fe_3Al$.

477. Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Foster Wheeler Development Corporation Contact J. L. Blough, (201) 535-2355

- The purpose of this project is to provide comprehensive corrosion data for selected advanced austenitic tube alloys in simulated coal ash environments.

478. Joining Techniques for Advanced Austenitic Alloys - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Tennessee Contact C. D. Lundin, (615) 874-5310

- The purpose of this research is to examine the welding and joining of advanced austenitic alloys.

479. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Argonne National Laboratory Contact K. Natesan, (312) 972-5103/FTS 972-5103

- The purpose of this task is to evaluate the corrosion mechanisms for chromia- and alumina-forming alloys in mixed-gas environments and to relate the mechanisms to mechanical property measurements.

480. Environmental Effects on Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact J. H. DeVan, (615) 574-4451/FTS 624-4451

- The purpose of this task is to develop protective oxide scales on $Al_20_3$-forming iron-based alloys in mixed oxidant environments.

481. Secondary-Ion Mass Spectrometry Study of Scales on Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; AEA Industrial Technology, Harwell Laboratory (England) Contact Hugh Bishop

- The purpose of this work is to analyze scales on iron aluminide alloys to determine the preferred diffusion paths of oxygen in these alloys.

482. Investigation of Moisture-Induced Embrittlement of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Rensselaer Polytechnic Institute Contact N. S. Stoloff, (518) 276-3476/FTS 624-4572

- The purpose of this work is to conduct experiments on selected $Fe_3Al$ alloys that will lead to an understanding of the moisture-induced embrittlement of iron aluminides.

483. The Effect of Alloying Constituents and Control of the Growth of Protective Oxide Scales -DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Battelle Columbus Laboratories Contact I. G. Wright, (614) 424-4377

- The objective of this program is to gain an improved understanding of the effects of alloying constituents present at low levels on the development and mode of breakdown of protective oxide scales in conditions representing those encountered in combustion and gasification processes.

484. Effect of Reactive Element Additions on the Protectiveness of Oxide Scales Formed in Sulfur-Containing Atmospheres - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Case Western Reserve University Contact K. M. Vedula, (216) 368-4211

- The focus of the current program is to obtain a better understanding of the effects of reactive element additions on the protectiveness of oxide scales formed in sulfidizing/oxidizing atmospheres.

485. Effects of Several Variables on the Growth and Breakdown of Protective Alumina or Chromia Scales in Mixed-Gas Environments -DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Universal Energy Systems, Inc., Contact V. Srinivasan, (513) 426-6900

- The main objective of this program is to develop a comprehensive basic understanding of the effects of additions of microalloy constituents and the surface conditions on the nucleation, growth and breakdown of protective oxide scales in the mixed oxidant environments relevant to coal utilization and conversion technologies.

486. Molten Salt-Induced Corrosion of Iron Aluminides - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Cincinnati Contact R. Y. Lin, (513) 556-3116

- The purpose of this project is to evaluate the molten salt-induced hot corrosion of iron aluminide alloys.

487. A Study of Erosive Particle Rebound Parameters - DOE Contacts J. P. Carr, (301) 353-6519; FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Notre Dame Contact T. H. Kosel, (219) 239-5642

- This research project is designed to provide a systematic investigation of the effects of materials properties and experimental variables on the rebound directions and velocities of erodent particles.

488. Studies of Materials Erosion in Coal Conversion and Utilization Systems - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Lawrence Berkeley Laboratory Contact A. V. Levy, (415) 486-5822

- The purpose of this project is to gain an understanding of the mechanisms by which metals and their corrosion scales lose material from their surfaces in the erosive wear environments typical of fluidized-bed combustion systems.

489. Response of Metallic and Oxide Surfaces to Deformation -DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact J. R. Keiser, (615) 574-4453/FTS 624-4453

- This task is directed at an understanding of the deformation response of metallic and oxidized surfaces.

490. Study of Particle Rebound Characteristics and Material Erosion at High Temperatures - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; University of Cincinnati Contact W. Tabakoff, (513) 475-2849

- The purpose of this effort is to investigate the erosion processes and fluid mechanics phenomena that occur in fluidized-bed combustors, coal-fired boilers, cyclones, pumps, turbines, valves, and other coal combustion systems.

491. Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Argonne National Laboratory Contact W. A. Ellingson, (312) 972-5068/FTS 972-5068

- The purpose of this project is to develop nondestructive evaluation techniques to characterize structural ceramics and detect flaws in early stages of processing as well as in the final densified state, and to correlate the presence of flaws to fracture behavior.

492. Joining of Silicon Carbide Reinforced Ceramics - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Idaho National Engineering Laboratory Contact B. H. Rabin, FTS 583-0058

- The purpose of this project is to identify and to develop techniques for joining silicon carbide fiber-reinforced composite materials.

493. Nondestructive Evaluation of Advanced Ceramic Composite Materials - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Idaho National Engineering Laboratory Contact L. A. Lott, FTS 583-6436

- The purpose of this project is to develop nondestructive evaluation methods to characterize the properties of advanced ceramic composite materials.

494. Structural Reliability and Damage Tolerance of Ceramic Composites - DOE Contact J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; National Institute of Standards and Technology Contact E. R. Fuller, (301) 975-5795

- The objective of this study is to characterize the high temperature failure mechanisms and factors that influence their operation with an aim toward improving the properties of structural ceramics, especially silicon carbide and silicon nitride based materials, for use in coal conversion applications.

495. Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; North Carolina A&T State University Contact J. Sankar, (919) 334-7620

- The purpose of this project is to expand the mechanical properties data base for composites fabricated by forced chemical vapor infiltration (CVI).

496. Ceramic Catalyst Materials: Hydrous Metal Oxide Ion Exchange Supports for Direct Coal Liquefaction - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Sandia National Laboratory Contact D. H. Doughty, FTS 845-8105

- This project involves investigation of the role of ceramic materials properties in the activity and selectivity of novel catalytic materials.

Device or Component Fabrication, Behavior or Testing

497. *Materials and Components in Fossil Energy Applications* (Newsletter) - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Battelle-Columbus Laboratories Contact I. G. Wright, (614) 424-4377

- The purpose of this task is to publish a periodic (bimonthly) newsletter to address current developments in materials and components in fossil energy applications.

498. Mechanisms of Galling and Abrasive Wear - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; National Institute of Standards and Technology Contact L. K. Ives, (301) 975-6013

- This project is directed to developing an understanding of the wear mechanisms of materials associated with valves in coal conversion systems.

499. Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition - DOE Contact J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; 3M Company Contact T. Kafka, (612) 733-8065

- The purpose of this project is to scale-up the chemical vapor infiltration and deposition (CVID) process developed at Oak Ridge National Laboratory for fabricating ceramic fiber-ceramic matrix composites. The goal is to use this scaled-up CVID process to produce composite filters.

500. Development of Ceramic Membranes for Gas Separation - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge Gaseous Diffusion Plant Contact D. E. Fain, (615) 574-9932/FTS 624-9932

- The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification.

501. Investigation of the Mechanical Properties and Performance of Ceramic Composite Components - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Virginia Polytechnic Institute and State University Contacts K. L. Reifsnider and W. W. Stinchcomb, (703) 961-5316

- The purpose of this project is to develop a test system and test methods to obtain information on the properties and performance of ceramic composite materials.

502. Material Data Base Development for Refractories - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Massachusetts Institute of Technology Contact Oral Buyukozturk, (617) 253-7186

- The objective of this project is to generate and compile experimental data on the thermomechanical behavior of selected high-chromia and high-alumina refractories.

503. Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Pacific Northwest Laboratory Contact J. L. Bates, (509) 375-2579

- The objective of this research is to identify and develop advanced materials for use as alternative electrodes and current interconnections in solid oxide fuel cells.

504. Gas Separations Using Inorganic Membranes - DOE Contacts L. A. Jarr, FTS 923-4555 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact B. Z. Egan, (615) 574-6868/FTS 624-6868

- The objective of this project is to explore the applicability of inorganic membranes to separate gases at high temperatures and/or in hostile process environments encountered in fossil energy conversion processes such as coal gasification.

505. Ceramic Fiber-Ceramic Matrix Hot-Gas Filters - DOE Contacts N. Holcombe, FTS 923-4829 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact D. P. Stinton, (615) 574-4556/FTS 624-4556

- This task will develop ceramic fiber-ceramic matrix materials and fabrication techniques suitable for production of hot-gas cleanup filters.

506. Identification of Materials for Hot-Gas Filter Tubesheets - DOE Contacts V. Kothari, FTS 923-4505 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. W. Swindeman, (615) 574-5108/FTS 624-5108

- The objective of this work is to assess current tubesheet designs and blowback manifold materials for ceramic crossflow and ceramic candle filters.

Instrumentation and Facilities

507. Management of the Fossil Energy AR&TD Materials Program - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- The purpose of this task is to manage the Fossil Energy AR&TD Materials Program in accordance with procedures described in the Program Management Plan approved by DOE.

508. Materials Specialist Assignment - DOE Contacts J. P. Carr, (301) 353-6519/ FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact R. R. Judkins, (615) 574-4572/FTS 624-4572

- This task involves the assignment of a materials specialist to DOE Fossil Energy to serve as a liaison between the Office of Technical Coordination and the AR&TD Materials Program Offices in Oak Ridge, Tennessee.

509. Coal Conversion and Utilization Plant Support Services - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contact J. R. Keiser, (615) 574-4453/FTS 624-4453

- This objective of this task is to provide support to the staffs of the DOE Energy Technology Centers and of operating coal conversion and utilization facilities in the areas of materials testing, evaluation, selection, and failure analysis.

510. Assessment of Fossil Energy Materials Research Needs - DOE Contacts J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735 National Institute of Standards and Technology Contact S. J. Dapkunas, (301) 975-6119

- The purpose of this activity is to identify long-range materials research and development needs and opportunities as they impact evolving fossil energy technologies.

Office of Coal Technology

The Office of Coal Technology is responsible for management of cooperative agreements with industry to foster clean coal technology; for the conduct of research and development programs for coal combustion and conversion, embodying retrofit or near-or mid-term applications such as fluidized-bed combustion and surface coal gasification; and for environmental, health and safety technology integral to such coal combustion and conversion systems.

Division of Clean Coal Technology

Instrumentation and Facilities

511. Materials Technical Support for the Clean Coal Program - DOE Contacts R. Santore, FTS 723-6131 and E. E. Hoffman, (615) 576-0735/FTS 626-0735; Oak Ridge National Laboratory Contacts R. R. Judkins, (615) 574-4572/FTS 624-4572 and J. R. Keiser, (615) 574-4453/FTS 624-4453

- This task is to provide materials technical support services to the projects on the Clean Coal Program which are being managed by the DOE Pittsburgh Energy Technology Center (PETC).

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# PARAGRAPH DESCRIPTIONS

# OFFICE OF BUILDING TECHNOLOGIES

## Office of Building Energy Research

The Office of Building Energy Research works to increase the energy efficiency of the buildings sector through performance of R&D on building systems and building equipment. In addition, 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

## Building Systems and Materials Division

The goal of this Division is to provide a scientific and technical basis (including model standards) for reducing the use of energy in residential and commercial buildings by 35 percent by the year 2000 from that used in 1975, while maintaining existing levels of human comfort, health and safety. The Division's primary objectives are to support research that advances the scientific and technical options for increased energy efficiency in buildings, to promote the substitution of abundant fuels for scarce fuels in buildings, and to promulgate standards for increased efficiency of energy use. To accomplish a portion of this, the Building Materials Program seeks to develop new and improve existing insulating materials; to develop and verify analytical models that are useful to building designers and researchers for predicting the thermal performance characteristics of materials; to develop methods for measuring the thermal performance characteristics; and to provide technical assistance and advice to industry and the public. The DOE contact is Peter Scofield, (202) 586-9193.

Materials Properties, Behavior, Characterization or Testing

1. Unguarded Thin Heater Tester — FY 1990 $150,000

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

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

2. Energy Savings with Advanced Building Materials — FY 1990 $150,000

DOE Contact: Peter Scofield, (202) 586-9193
LBL Contact: Ron Kammerud, (415) 486-6620

This project is for the identification and quantification of the energy saving potentials of commercial buildings using advanced materials. The four generic classes of materials being analyzed are: high R-value (>100) insulations, variable (switchable) R-value insulations, selective surface coatings and switchable emissivity films. The results of this analysis will be used as a guide for the allocation of program resources and to establish technical performance objectives for the development of new advanced materials.

Keywords: Active Thermal Insulation, Switchable Emittance, Energy Savings Calculation

3. Recommended R-Levels - ZIP Program — FY 1990 $40,000

DOE Contact: Peter Scofield, (202) 586-9193
NIST Contact: Steve Petersen, (301) 975-6136

This effort has two parts. First to provide minimum recommended R-values for residences for inclusion in the DOE Insulation Fact Sheet. These values are based on climate identified by Zipcode and on regional average values of insulation costs and space heating and cooling costs. The second is to update the ZIP computer program used to provide the recommendations, to include slab floors, cathedral ceilings, ductwork and water heaters. This Fact Sheet and the ZIP program Version 2.0 are now available for use by the building conservation community.

Keywords: Recommended R-Values, Computer Program, Economic Analysis, Economic Analysis

4. CFC Foam Characterization FY 1990
$70,000

DOE Contact: Peter Scofield, (202) 586-9193
NIST Contact: H. Fanney, (301) 975-5864

This effort is to determine the effect of variations in thermal conductivity and test specimen thickness in calibrating the R-matic and K-matic apparatuses used in the foam insulation industry to measure the therm conductivity of rigid foam insulations.

Keywords: Insulation Sheathing, Walls, Roofs, Economic Analysis

5. Foam Insulation Research FY 1990
$75,000

DOE Contact: Peter Scofield, (202) 586-9193
MIT Contact: Leon Glicksman, (617) 253-2233

Freon-blown rigid urethane foam insulation is being investigated to determine the degree to which the effective thermal conductivity decreases with time. Various types of reflective flakes are also being investigated for their effectiveness in lowering the thermal conductivity of foam insulations.

Keywords: Building Insulation, Heat Transfer, Radiation

6. Development of Non-CFC Foam Insulations FY 1990
$100,000

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

This a three year joint project with the rigid foam industry and EPA for the development of alternative blowing agents to be used as drop in replacements for the CFC blowing agents currently being used in the manufacture of foam insulation products. Prototype rigid foam boards with five different blends of HCFC-123 and 141b will be manufactured by industry and sent to ORNL for testing and evaluation both in the laboratory and in outdoor test facilities. Tests will be conducted to determine mechanical and thermal properties and aging characteristics.

Keywords: CFC, Foam Insulation, Insulation Sheating, Roofs

7. Compact Vacuum Insulation — FY 1990 $125,000

DOE Contact: Peter Scofield, (202) 586-9193
SERI Contact: Tom Potter, (303) 231-1083

This advanced technology insulation project is for the development of a vacuum insulation concept. Two thin stainless sheets are welded together at the edges and a hard vacuum is drawn in the cavity between the sheets separated by matrix of small glass spheres. Panels with center R-values of five have been made that are 0.1 inches thick. The project goal is to improve center R-values to fifteen.

Keywords: Insulation, Vacuum, Heat Transfer, Radiation

8. Evacuated Powder Panel Insulation — FY 1990 $150,000

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

This project is for the development of an advanced technology super insulation concept. A layer powder is sandwiched between two films and a soft vacuum is drawn on the powder filler. Current technology produces a R-20 per inch panel. Improved powders and longer life encasing films are being developed.

Keywords: Insulation, Vacuum, Heat Transfer

# OFFICE OF INDUSTRIAL TECHNOLOGIES

This Office supports a broad range of research, including long-term, high-risk, high pay-off R&D in the Advanced Industrial Concepts Division to shorter-term engineering in other divisions. Cost-shared research and development for industrial energy conservation technologies that offer large potential for saving scarce fuels is promoted. 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.

## Office of Waste Reduction Technologies

Waste 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 office conducts research to develop advanced waste energy recovery technologies for the industrial sector.

## Industrial Energy Efficiency Division

### Materials Properties, Behavior, Characterization or Testing

9. Advanced Heat Exchanger Material Technology Development — FY 1990 $445,000

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

This project conducts research to develop improved ceramic materials and fabrication processes and to expand the materials data base for advanced heat exchangers. Currently the project is studying the effects of corrosive waste stream constituents on candidate ceramic and ceramic composite materials through coupon tests and exposure to synthetic-exhaust streams, conducting scale-up studies on the carbo-thermic production of $\beta$-SiC powder, and developing advanced wet forming techniques for monolithic ceramic components.

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

10. Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components — FY 1990 $200,000

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: J. Bower, (804) 522-5742

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

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

11. National Laboratory Support to Assessment of Strength Limiting Flaws in Ceramic Heat Exchanger Components — FY 1990 $63,000

DOE Contact: S. Richlen, (202) 586-2078
Idaho National Engineering Laboratory Contact: W. Reuter, (208) 526-1708

This project supports the B&W study on strength limiting flaws by the development of advanced NDE, test methods, and other key technologies. Currently the project is studying the application of Moire Interferometry to measure stress of components under test.

Keywords: Structural Ceramics, NDE, Structure

12. Ceramic Fiber Residue Measurement — FY 1990 $ 0

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

This project determines whether whisker-like particles can be generated during the handling, processing, or machining of continuous ceramic fiber ceramic matrix composites. Currently a test protocol is being written.

Keywords: Ceramic Composites, Whiskers

13. Characterization of Beta Alumina for a Sodium Heat Engine Application

FY 1990
$460,000

DOE Contact: W. Parks, (202) 586-2093
ANL Contact: R. Valentin, (708) 972-4493

This project is a materials characterization study to determine if the current beta alumina tubes used in the sodium heat engine are of sufficient quality to perform adequately in service. The study will examine the stress levels in commercial tubes using mechanical testing, NDE, and new NMR process. Preliminary work on improved processing methods are being examined.

Keywords: Beta Alumina, Sodium Heat Engine, AMTEC, NDE of Ceramics

Device or Component Fabrication, Behavior or Testing

14. Ceramic Composite Heat Exchanger for the Chemical Industry

FY 1990
$ 0

DOE Contact: S. Richlen, (202) 586-2078
Babcock & Wilcox Contact: D. Hindman, (804) 522-5825

This second phase of this project which addressed critical problems of the material and design has been completed. Alumina fiber in a zirconia or alumina oxide matrix has been selected as most promising material. Currently, the field test host site has been selected and final design is being conducted.

Keywords: Ceramic Composites, Structure

15. HiPHES System Design Study for Energy Production from Hazardous Wastes

FY 1990
$465,000

DOE Contact: S. Richlen, (202) 586-2078
Solar Turbines Contact: B. Harkins, (619) 544-5398

This project has completed the first phase of a three-phase effort to develop high pressure heat exchange systems for recovery of energy from hazardous wastes. A preliminary design of an advanced heat exchange process based on the use of ceramic composites has been developed. Research on critical material and design needs will now begin.

Keywords: Ceramic Composites, Heat Exchangers

16. HiPHES System Design Study for an Advanced Reformer FY 1990 $800,000

DOE Contact: S. Richlen, (202) 586-2078
Stone & Webster Engineering Corp. Contact: J. Williams, (617) 589-7147

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

Keywords: Composites, Heat Exchangers

17. Ceramic Components for Stationary Gas Turbines in Cogeneration Service FY 1990 $355,000

DOE Contact: W. Parks, (202) 586-2093
Battelle Contact: D. Anson, (614) 424-5823

This project examines the state of the art in ceramic components for turbine engines, current stationary gas turbine design and economics, and projects a plan to introduce ceramics into stationary gas turbines.

Keywords: Structural Ceramics, Cogeneration, Gas Turbines

Waste Material Management Division

Waste Utilization and Conversion

Industrial waste solid, liquid, and gaseous materials are waste because they have insufficient economic potential, thus they are landfilled or discharged to the environment. Economically useful wastes are termed by-products and constitute the objective of the Waste Utilization and Conversion program. Materials research can provide technologies to upgrade wastes or create new commodity materials so that wastes can have economic, i.e., added, value to become by-product materials of value to industry or commerce. The DOE contact is Jerome Collins (202) 586-2369.

Materials Preparation, Synthesis, Deposition, Growth or Forming

18. Wood Wastes to Adhesives — FY 1990 $545,000

DOE Contact: Alan Schroeder, (202) 586-1641
SERI Contact: Helena Chum, (303) 231-7249

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

Keywords: Wood, Wastes, Adhesives, Pyrolysis

19. Waste Rubber-Polymer Composite — FY 1990 $417,000

DOE Contact: Stuart Natof, (202) 586-2370
Air Products & Chemicals, Inc., Contact: Dr. Bernard Bauman, (215) 481-6053

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

Keywords: Tires, Composites, Surface Activation

20. Zinc-Contaminated Steel Conversion — FY 1990 $150,000

DOE Contact: Stuart Natof, (202) 586-2370
Argonne National Laboratory Contact: Edward J. Daniels, (708) 972- 5279

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

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

21. Silicon Oxide Recovery-Conversion

FY 1990
$851,000

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

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

Keywords: Silicon Oxide, Waste Recovery, Waste Conversion

22. Waste Food Carbohydrates to Lactide Copolymer Plastics

FY 1990
$500,000

DOE Contact: Alan Schroeder, (202) 586-1641
Argonne National Laboratory Contact: Robert Coleman, (708) 972-3268

A process is being developed with TVA, States of Illinois and Minnesota, to produce a biodegradable mulch film/coating with time release fertilizer and pesticide properties that does not have to be taken up at the end of the growing season. An energy analysis indicates savings of 55,000 Btu/lb of plastic used, with a large potential market. It also provides a higher value product outlet for such carbohydrate wastes as cheese whey, potato processing, and corn processing.

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

Solar Materials Research

The objective of solar materials research is to identify and develop viable materials processes that take advantage of the attributes of highly concentrated solar fluxes. Solar technology is able to supply concentrated radiant energy to surfaces with high efficiency and without many of the environmental liabilities of conventional power supplies.

Materials Preparation, Synthesis, Deposition, Growth or Forming

23. Materials Processing Using High Solar Photon Flux — FY 1990 $500,000

DOE Contact: Frank Wilkins, (202) 586-1684
SERI Contact: Meir Carasso, (303) 231-1353

Metalorganic precursors for the yttrium-barium-copper-oxide (YBCO) group of superconductors were spin-coated onto single crystal yttrium stabilized zirconia ($ZrO_3$) and magnesium oxide (MgO) substrates, dried in air, then thermally processed in oxygen using the solar furnace at SERI. Zero resistivity was measured at 74.7K. It is likely that the higher deposition rates and high heating rates made possible by the solar furnace will enable better economics for existing superconductivity films as well as new films to be developed.

Thin films of carbon have been grown on Ni and Si substrates using $CH_4$ and $H_2$ as precursors. The carbon growth on Ni results in a graphitic phase. Experiments with Si substrates have produced thin films of SiC and diamond-like carbon films, as well as graphitic carbon, depending upon the growth conditions. Current technology using microwave plasmas or hot filaments requires using large amounts of energy to grow diamond thin films.

Work is continuing on a variety of surface deposition techniques to obtain special properties and on surface modification of alloys.

Keywords: Solar Furnace, Superconductors, Diamond-like Carbon, Diamond Films

24. Catalysts for Solar-Assisted Water Detoxification — FY 1990 $500,000

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

Titanium dioxide (anatase form) acts as a photocatalyst for the oxidation of hazardous organic compounds in contaminated water. In order to improve the efficiency of the solar water detoxification process, research is directed toward increasing the overlap of the action spectrum of the photocatalyst with the solar spectrum and increasing the efficiency of conversion of photons to active oxidizing species on the catalyst.

Keywords: Titanium Dioxide, Water Treatment, Water Purification, Photocatalyst, Semiconductor

Office of Industrial Processes

This office 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.

Improved Energy Productivity Division

Materials Preparation, Synthesis, Deposition, Growth or Forming

25. Composite Cathode Material Development FY 1990 $910,000

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

This is a long term project involving testing and analysis of composite materials for cathode applications. During FY 1990, work was completed on finite element analysis of $TiB_2$-graphite samples and engineering calculations for a commercial cell heat balance in order to optimize shapes and structures. The project has been moved to the metals initiative.

Keywords: Composites, Cathode

26. Cerox Inert Anode Material FY 1990 $460,000

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

The addition of $CeO_2$ to molten cryolite produces a coating on oxygen evolving electrodes. The factors controlling the in situ formation of the coating, the coating characteristics, and the coating stability have been evaluated. Metal purity and voltage drops will be determined for commercial aluminum reduction cell operating conditions.

Keywords: Coatings, Anode, Ceramics

27. Lightweight Alumina Aggregate FY 1990 $ 0

DOE Contact: M. J. McMonigle, (202) 586-2082
Alcoa Contact: Al Pearson, (412) 337-2706

Completed literature search and initiated bench scale experiments for manufacture of new lightweight aggregate composition.

Keywords: Insulating Refractories

28. High Temperatures Fiber Insulation FY 1990 $ 0

DOE Contact: M. J. McMonigle, (202) 586-2082
Manville Contact: Phil Martin, (303) 478-5252

Phase I was initiated to systematically characterize commercially available refractory fibers for thermal, physical, and refractory stability properties. A literature search was completed and computer codes enhanced to calculate heat loss and heat storage properties for specified furnace configuration.

Keywords: Insulating Refractories

Materials Properties, Behavior, Characterization or Testing

29. Expand and Control Inert Electrode Cell Operating Conditions FY 1990 $362,000

DOE Contact: M. J. McMonigle, (202) 586-2082
PNL Contact: Larry Morgan, (509) 375-3874

Digital signal analysis and chaos theory are being applied to determine alumina concentration at saturation in operating electrolytic cells in real time.

Keywords: Ceramics, Cryolite, Material Science, Aluminum

Advanced Industrial Concepts Division

The mission of AICD is to support generic, long-term, high-risk applied R&D in those processes and technologies that underpin industrial unit operations. The AICD output provides a technology base to improve energy use efficiency and advance industrial capability to use alternative energy resources. Materials-related research in AICD is conducted in the Advanced Industrial Materials (AIM) Program. The AIM Program develops generic materials technologies brought to a stage for private industry or other government programs to advance further towards technology and engineering demonstration. The Program emphasizes materials as an enabling technology for industrial energy conservation and focuses on six areas: Structural Engineering Materials, Thermally Insulating Materials, Other Unique Materials (entirely superconducting ceramics at this time), Innovative Processing Technology, Lightweight and Biobased Materials (principally plastics recycling and environmental compatibility), and Materials System Reliability. The acting Program Manager is Marvin E. Gunn, (202) 586-5377.

Materials Preparation, Synthesis, Deposition, Growth or Forming

30. Aerogel Thermal Insulators

FY 1990
$300,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
LBL Contact: Arlon Hunt, (415) 486-5370

The objective of this research project is the development and production of controlled porosity materials with tailored thermal, optical, and physical characteristics. This effort is a combined program of analytical studies and experimental measurement of the particle creation and assembly process. In addition, the properties of the finished material will be determined and related to the preparation technique.

Keywords: Thermal Insulation, Sol-Gel, Processing

31. Chemical Vapor Deposition of Ceramic Composites

FY 1990
$850,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contact: Peter Angelini, (615) 574-4565
SNL-L Contact: Mark Allendorf, (415) 294-2895
Thermoelectron Technologies Contact: Peter Reagan, (617) 622-1347

The objective of this effort is to explore novel ceramic matrix composites produced by simultaneous chemical vapor deposition (CVD) of a dispersoid phase and a matrix phase. The basic mechanisms which control the toughness, strength, thermal expansion, and thermal conductivity of the composite coatings are investigated by varying the quantity, composition, and morphologies of the two phases.

The ultimate objective is to utilize the CVD process to fabricate ceramic matrix composites, stable in air at 2500 °F with 30 ksi fracture strength and 10 MPa $\sqrt{m}$ fracture toughness and thus develop a single step process for fabrication of ceramic composites which are stable in air at high temperatures, and will have numerous applications in automotive and gas turbine engines, chemical processing and waste heat energy.

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

32. Thin-Wall Hollow Ceramic Spheres from Slurries FY 1990 $150,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contact: David L. McElroy, (615) 574-5976
Georgia Institute of Technology Contact: J. Cochran, (404) 894-6104

This effort is investigating the development of processes for economically fabricating hollow thin-wall spheres from conventional ceramic powders using dispersions and is assessing their potential use. Initially successful production of spheres of $Al_2O_3$ and $Al_2O_3Cr_2O_3$ was followed by experimental assessment of the structural and thermal insulation potential for these unique low density materials using both simulated models and experimental measurements. Georgia Tech will continue to assess the structural capability of the spheres and, together with ORNL, evaluate the feasibility of using pacifiers to reduce high temperature thermal conductivity.

A commercial company, Ceramic Filler Inc., is operating a pilot plant in Atlanta, Georgia, and a production facility (capacity 800 tons/year) in South Carolina.

Transfer of this technology will bring a potential payoff of a high temperature insulating material with less cost, higher thermal efficiency, and without ecological and health dangers.

Keywords: Structural Ceramics, High Temperature Service, Insulation

33. The Role of Inert Gas Entrapped in Rapidly Solidified Materials FY 1990 $700,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
INEL Contact: John Flinn, (208) 526-8127
SNLL Contact: W. G. Wolfer, (415) 294-2307

This investigation seeks to determine property modifications, including enhanced microstructural stability and strengthening, for rapidly solidified materials containing entrapped inert gases. The approach is both experimental and theoretical with initial work on nickel-base alloys.

It has been determined that rapid crystallization during powder atomization provides a supersaturation of vacancies in the form of nanosized clusters that are stabilized by internal oxidation to 0.9 $T_m$ and responsible for the observed high temperature strengthening.

The applicability of rapid solidification processing to superalloys will be investigated in FY90.

Keywords: Gases in Metals, Rapid Solidification

34. Biobased Materials - Composites

FY 1990
$150,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
SERI Contact: Helena Chum, (303) 231-7249
University of Wisconsin Contact: Ray Young, (608) 262-0873
U.S. Forest Products Laboratory Contact: Roger Rowell, (608) 264-5816
University of Southern Mississippi Contact: Lon Mathias, (601) 266-4868
Virginia Polytechnic Institute & State University Contact: Wolfgang Glasser, (703) 231-4403

The overall objective of this effort is to develop cost-effective and environmentally compatible materials for composites and other materials for the automotive industry that incorporate high levels of inexpensive renewable polymers, but have strength properties of synthetic materials and have good overall properties, including low cost. Current work is emphasizing assessing chemical modifications of wood and wood components from inexpensive wood fractionation routes to produce materials for the automotive industry. Renewable materials are lightweight, corrosion resistant and have sound deadening properties. These properties make them well-suited for automotive applications. Strength properties, principally impact strength, need to be improved.

The approach involves tailoring of plastics properties with the design of specific chemical modifications of the wood materials. Some modifications impart thermoplasticity directly; others improve physical properties such as dimensional stability. Approaches that use non-woven technologies and wood fibers as reinforcing agents for composites are investigated. The non-woven mats can be molded into specific shapes that lead to parts consolidation and avoid multiple stamping operations used to fabricate these parts from steel.

Keywords: Composites, Biodegradable Plastics, Natural/Synthetic Resins

35. Microwave-Driven Spray Drying — FY 1990 $350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
LANL Contacts: F. Gac, (505) 667-5126

The objective of this effort is to develop a generic micro-driven spray drying process for the aerosol preparation of fine, homogeneous powders in complex metal oxide systems. Microwave powder shall be coupled directly to the mist of aqueous or organic solutions of metal compounds, and will heat the mist to drive off the solvent leaving a fine powder of a complex metal compound. Given sufficiently high evaporation rates, a very homogeneous powder will result directly from solutions of metal nitrates, chlorides, etc. Although the focus will be on the synthesis of complex metal oxide powders, the process is conceivably applicable to any application that utilizes spray drying.

Keywords: Microwave Processing, Spray Drying, Powder Synthesis

36. Magnetic Field Processing of Polymers — FY 1990 $350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
INEL Contact: Alan Donaldson (508) 526-2627/FTS 583-2627
LANL Contact: Gerald Maestas, (505) 667-3973/FTS 843-3973

The objective of this task is to demonstrate and model the effects of an applied magnetic field during processing of inorganic or organic polymers in order to improve their physical, mechanical, and separation capabilities. Quantitative correlations will be made between the physical properties of materials prepared with and without the presence of applied magnetic fields.

Keywords: Magnetic Field, Polymers, Inorganic, Organic

37. Electrochemical Synthesis of Conducting Polymers and Electrocatalysts — FY 1990 $800,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
LANL Contacts: Gerald Maestas, (505) 667-3973/FTS 843-3973 and S. Gottesfeld, (505) 667-0853

The objectives of this task are to: 1) develop electrochemical techniques for the synthesis and analysis of conducting polymers in order to improve the composition, morphology, and stability of conducting polymer films for applications including corrosion resistant conductive coatings and electrochromic films and 2) develop new methods to fabricate low cost platinum electrocatalysts with a particle size of less than 2 nm in average diameter by ion-exchange techniques.

Keywords: Catalyst, Polymer, Electrical Conductivity

38. Polymers with Improved Surface Properties — FY 1990 $100,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contact: Peter Angelini, (615) 574-4565 and L. K. Mansur, (615) 574-4797
LANL Contact: Gerald Maestas, (505) 667-3973/FTS 843-3973

The objective of this task is to develop innovative technology for surface modification of polymers to produce smooth, hard, corrosion resistant for applications requiring lightweight and improved properties. The surface of polymers will be modified by the use of multiple ion beam treatments and plasma processing. The microstructure will be related to processing conditions and properties.

Keywords: Polymers, Surface Modification, Ion Beam

Materials Structures and Composition

39. Modeling and Development of Ordered Intermetallic Alloys — FY 1990 $1,200,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
LANL Contact: A. D. Rollett, (505) 667-6133/FTS 843-6133
ORNL Contacts: Peter Angelini, (615) 574-4565, C. T. Liu, (615) 574-4459, V. K. Sikka, (615) 574-5112, M. L. Santella, (615) 574-4805 and D. M. Nicholson, (615) 574-5873
Imperial College (U.K.) Contact: D. G. Pettifor, 011-411-589-5111, ext. 5756

The ultimate objective of this effort is the development of the mathematical models and research software for use in the design of materials for energy technology applications. During FY 1990 emphasis was shifted from modeling the Ni-Al systems to modeling and confirmation laboratory testing of $MoSi_2$. To date, modeling efforts have related the role of boron at grain boundaries in $Ni_3Al$ and found agreement with subsequent experiment.

$MoSi_2$ represents an attractive material for high temperature applications (high melting point, oxidation resistance, ductile above 900 °C), but brittle behavior at low temperature limits usefulness and provides a good field for improvement when addressed by a combination of modeling and experiment.

Keywords: Intermetallic Alloys, Modeling of Materials

40. <u>Thermosetting Resins with Reversible Crosslinks</u> FY 1990
$150,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
Polytechnic of New York Contact: Giuliana Tesoro, (718) 643-5244

The objective of this effort is to determine if it is possible to develop thermosetting resins with "reversible crosslinks." If so, it may be possible to produce plastics with the strengths, toughness, temperature capabilities, and corrosion resistances typical of thermoset resins but which can be easily reprocessed like a thermoplastic. This process would allow easier recycling, thereby reducing the need for virgin plastics made from natural oil or gas as well as easing the repair of lightweight automotive structural parts.

In the initial phase of the project, the feasibility of the approach was demonstrated for an epoxy resin, crosslinked with disulfide-containing reagents, solubilized by reduction after curing, and thereafter crosslinked by oxidation or by reaction with bifunctional compounds. This sequence has been accomplished for commercial epoxy resins of higher molecular weight and of higher functionality. Evaluation of the thermal and mechanical properties of the crosslinked resins has shown that they are similar to, and, in some instances, superior to those of products crosslinked with commercial curing agents.

Experimental polyimides containing disulfide bonds have been prepared and it has been shown that, as in the case of epoxy resins, it is possible to solubilize cured resins by reduction, and to set the soluble products in a subsequent step.

Keywords: Thermoset Resins, Recycling Plastics

41. <u>Biobased Materials - Packaging Plastics</u> FY 1990
$350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
SERI Contact: Helena Chum, (303) 231-7249
Michigan Biotechnology Institute Contact: Ramani Narayan, (517) 349-2970

Research in this area will attempt to develop cost-effective and environmentally degradable packaging plastics that incorporate high levels of inexpensive renewable polymers, but have strength properties of synthetic thermoplastics.

During FY 1990 assessments were made of the suitability of starch/polystyrene graft copolymers for compatibilizing starch and polystyrene plastics at low concentration levels of the grafts, while maintaining the physical properties of the synthetic plastics in the resulting ternary alloys (starch, polystyrene, and graft copolymer).

Keywords: Packaging, Plastics, Copolymers

42. Innovative Approaches to the Chemical Recycling of Plastics — FY 1990 $500,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
SERI Contacts: Helena Chum, (303) 231-7249 and Robert Evans, (303) 231-1384

This research activity is aimed at developing cost-effective and environmentally benign processes for recovering mixed plastics from various sources, such as auto-shredder waste, carpet waste, and other source-separated mixed plastic streams.

Current effort is directed at the identification of experimental conditions for the chemical recovery of a high proportion of monomeric and other high-value components from plastics mixtures using advanced thermal processes.

The SERI molecular-beam mass spectrometer is being used to detect real time products of these processes and establish conditions that will accomplish the ultimate objective of small-scale experiments.

Keywords: Plastics Recycling, Pyrolysis

43. Recycling of Sheet Molding Compounds — FY 1990 $0

DOE Contact: Marvin E. Gunn, (202) 586-5377
Stevens Institute of Technology Contact: K. E. Gonsalves, (201) 420-5779 and S. S. Stivala, (201) 420-5529

The ultimate objective of this project is the development of final flow sheets and the assessment of the technical and economical feasibility of the proposed recycling process.

As a first step model polymers for recycling from a given class of commercially significant polymeric materials were selected. Thermoset composites (SMC) are widely used in the automotive industry (and elsewhere), so this class of materials was chosen.

In order to establish the parameters essential for economically converting discarded thermoset composites (such as SMC) to useful products, two basic types of operations are necessary: mechanical operations (chopping, grinding and filtration); and chemical processes (solvent extraction, hydrolysis, separation). These were studied in detail.

Technical collaboration with General Motors, manufacturer of SMC based automotive components, and Ashland Chemical Co., sole supplier of the basic SMC ingredients package to GM, was established. Thus, SMC sheets, already compression molded, and polyester resins for PHASE ALPHA SMC were obtained from both GM and Ashland.

Within the next 5 to 10 years junkyards will be covered with SMC automobiles and trucks that cannot be scrapped and recycled in a manner similar to those made from metals. This study could reduce the bulk of the material for dumping and provide economic recovery of useful raw materials.

Keywords: Plastics Recycling, Pyrolysis

44. Laser Deposition of Thin Films for High Temperature Superconductors — FY 1990 $300,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contacts: Peter Angelini, (615) 574-4565, D. H. Lowndes, (615) 574-6306 and D. M. Kroeger, (615) 574-5155

The major objectives of this project are the development of pulsed laser deposition methods which will continuously deposit HTSC films on practical substrates followed by the transfer of the technology to the electric motor industry.

Pulsed laser deposition conditions have been found that result in high $J_c$ (>1 MA/cm $^2$), high $T_c$ (~92 °K) $YBa_2Cu_3O_{7-x}$ films formed on single crystal substrates. Rapid, low temperature post deposition oxidation, resulting in fully oxidized $YBa_2Cu_3O_{7-x}$ films, has been demonstrated and investigations of the influence of substrate polycrystallinity and substrate surface preparation on film morphology are underway.

During FY89 work concentrated on production of thin films and composites of 123-YBaCuO with silver and the development of microstructures capable of high critical current density and superior mechanical properties.

Keywords: Laser Deposition, Thin Films, HTSC

45. Microwave Sintering and Joining of Advanced Ceramics (Zirconia-Toughened Alumina (ZTA) and Microwave Joining of Ceramics) FY 1990 $600,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contacts: Peter Angelini, (615) 574-4565 and Ron Beatty, (615) 574-4536
Technology Assessment and Transfer, Inc., Contact: R. Silberglitt, (301) 261-8373

In both HTSC Materials studies and in the ZTA research area a major objective was to evaluate the effectiveness of microwave sintering as opposed to conventional sintering techniques. HTSC activities were aimed at developing a technically superior, cost effective method for manufacturing high temperature superconductors. Densification behavior and superconducting properties of both microwave and conventionally sintered superconductors using powders from commercial industry and in-house sources were studied. Densification was very different for different powders but only slightly affected by microwave versus conventional sintering. Superconducting properties showed some differences but not major improvement from microwave sintering.

The objective of ZTA sintering research was to assess microwave effects on the kinetics of grain growth in alumina in order to understand the controlling parameters and then to develop a method for fabricating high toughness ZTA from low cost materials. To date it has been found that kinetics of grain growth are much higher for microwave heating than conventional heating; rate of grain growth, for microwave at 1500 °C was the same as that for conventional heating at 1700 °C. Found densification of alumina with 20 wt % zirconia occurred 300-400 °C lower for microwave sintering compared with conventional sintering.

In microwave joining of ceramics the objective was to demonstrate the applicability of the technique to materials of industrial interest and under conditions relevant to industrial processing, and develop application projects in collaboration with industry.

A single-mode, tunable rectangular cavity has been integrated with a hydraulic press, IR pyrometer, forward and reflected power probes, and *in situ* acoustic NDE. A separate apparatus using a cylindrical resonant cavity and a frequency sweeper was used to measure dielectric properties of candidate materials.

Theoretical feasibility was demonstrated. An experimental system was constructed which verified the microwave heating model. Alumina-glass-alumina joints were made. Mullite-to-mullite joints were made without surface preparation or interlayer. These demonstrated that the joints are stronger than the base material. Novel instrumentation for dielectric properties and *in situ* NDE was developed. The capability to perform experiments in nitrogen or inert gas environment was added. Current focus is on applying the technique to alumina (ECUT funding) and proprietary materials submitted by industry (corporate sponsorship).

Keywords: Microwave, Sintering, HTSC, Zirconia, Alumina, Ceramic Joining

46. Biomimetic Thin Film Ceramic Coatings — FY 1990 $300,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
PNL Contact: Gary McVay, (509) 375-3762

The objective of this research is to develop energy-conserving, novel processing methods (mimicking natural or biological processes) for the nucleation and growth of ceramic oxide thin films onto metal, ceramic, and polymer surfaces from aqueous solutions.

This project is developing a new process for the formation of thin film materials. Mineral deposition from aqueous solutions is controlled by organized organic functional groups attached to the underlying substrate by appropriate coupling agents. Such derivatization eliminates dependence of the thin film growth process on the native substrate characteristics and allows a generalized scheme for thin film deposition to be developed.

The process under development closely follows the methods used by biological systems to grow hard (ceramic) tissue. As such, the process is very energy efficient. In addition, the devices developed from this unique process will contribute significantly to more efficient energy utilization. Applications will focus on protective coatings, sensors, and catalysts. Examples of the most realistic applications follow:

1. Protective coatings for corrosion or abrasion resistance.

2. Built-in or remote, industrial sensors (corrosion detectors or in-line chemical sensors for process control).

3. Catalytic surfaces for chemical and energy processes (hydrogenation, polymerization, cracking, or coal liquefaction).

4. Thin film coatings on radiant tiles or industrial gas burners.

Keywords: Mineral Deposition, Ceramic Coatings

Materials Properties, Characterization, Behavior or Testing

47. X-Ray Tomography for Ceramic Composites — FY 1990 $300,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
LLNL Contact: John Kinney, (415) 243-6669/FTS 532-6669

The objectives of this task are to develop the use of X-ray tomography to identify flaws, relate processing conditions to microstructure, and improve properties of crack resistant composites. The task will concentrate on the characterization of the micro- and macrostructure of fiber reinforced composites. The results will be used to correlate relationships between processing conditions such as temperature and gas composition on density and mechanical properties. Modeling will also be performed.

Keywords: X-Ray, Tomography, Composites

48. Variable Insulation Concepts — FY 1990 $150,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
SERI Contact: T. R. Penney, (303) 231-1754/FTS 327-1754

The objective of this task is to develop variably-insulating panels. The performance requirements and potential benefits will be defined in collaboration with end-user process industries. The technical feasibility of design concepts will be analyzed.

Keywords: Thermal Insulation

49. Ordered Intermetallic Alloys for Corrosion Resistance (FeAl Development)

FY 1990
$200,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contacts: Peter Angelini, (615) 574-4565 and C. T. Liu, (615) 574-4459

An initial objective in this area was the identification of an FeAl composition with the best combination of room temperature ductility, and corrosion resistance in oxidizing molten nitrate salt environments.

A binary base composition of FeAl was selected on the basis of tensile strength results, creep strength, fabricability and corrosion resistance. Minor alloying additions brought a room temperature tensile ductility greater than 10 percent. (This represents a five-fold increase in ductility compared to the pure binary aluminide.) FeAl compositions with excellent corrosion resistance in molten nitrate salts were also identified.

Future activities will include; alloy design to improve creep strength, while maintaining ductility; evaluation of resistance of FeAl compositions to high-temperature oxidation; a weldability study; and finally, scale-up to industrial size "heats" and further interactions with industry.

Keywords: Corrosion Resistance, Iron Aluminide

50. Characterization of SiC Whisker - $MoSi_2$ Composites for Elevated Temperature Applications

FY 1990
$800,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
LANL Contact: J. J. Petrovic, (505) 667-0125

SiC whisker-$MoSi_2$ matrix composites are being examined for potential elevated temperature structural applications in oxidizing environments.

Significant improvement in high temperature yield strength has occurred as a result of solid solution alloying of the matrix. At 1500 °C, composite yield strengths were 8-10 higher than pure $MoSi_2$, reaching values of 80 MPa in air testing. High temperature ductility and oxidation resistance were retained in the composites.

In FY90, project emphasis will shift to lowering the brittle-to-ductile transition of $MoSi_2$ by a Materials-by-Design approach, and the development of high toughness partially stabilized $ZrO_2$-$MoSi_2$ matrix composites. Technology transfer interactions with U.S. industrial organizations will continue.

$MoSi_2$ based composites constitute a new class oxidation-resistant high temperature materials which represent an alternative to structural ceramics.

Keywords: Intermetallic Alloy, Composites, Whiskers

Device or Component Fabrication, Behavior or Testing

51. Chemically Specific Coatings — FY 1990 $350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
SNLA Contact: G. C. Frye, (505) 844-0787

This project will attempt to develop a new class of chemically specific coatings that can be used in separations, waste recovery and as process monitors to improve process energy efficiency.

Sol-gel chemistry and surface modification techniques are used to develop oxide coatings with controlled pore sizes and tailored chemical properties. These films provide chemical selectivity based on both molecular size and chemical interactions.

Keywords: Coatings, Sol-Gel Processing

52. Development of High-Temperature Superconducting Magnets for High-Efficiency Motors and Power Electronics — FY 1990 $350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contacts: Peter Angelini, (615) 574-4565, D. H. Lowndes, (615) 574-6306 and R. A. Hawsey, (615) 574-8057

As part of this research effort, potential applications for HTSC magnets for motors, heat pumps, etc., are being identified and general design requirements for magnets in these applications are being developed.

Keywords: HTSC Films, Superconducting Magnets, Motor

53. Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets

FY 1990
$350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
PNL Contact: Larry R. Pederson, (509) 375-2731
Boeing Aerospace Contact: Thomas Luhman, (206) 234-2683

A preliminary goal of this project is the design and demonstration of a trapped-flux permanent magnetic device using bulk, polycrystalline superconducting ceramics in the BiSrCaCuO and/or TlBaCaCuO systems that have critical current densities of at least $10^5$ $A/cm^2$ at 77°K. Subsequently it is intended to improve the critical properties of bulk, polycrystalline superconducting ceramics so that they can be utilized in practical devices, including motors, generators, and switches.

Freeze-drying and aerosol pyrolysis processes will be used to prepare phase-pure, homogeneous, fine-grained, superconducting ceramics. The BiSrCaCuO and TlBaCaCuO systems were selected because of their high critical temperatures. Critical current densities in a magnetic field will be enhanced by doping the grain boundaries so that they become superconducting by a proximity effect, and by introducing secondary phase precipitates to act as flux pinning centers.

Keywords: Superconducting Magnets, High Temperature Superconductors, HTSC

Facilities

54. Multiple Frequency Microwave Energy Source and Furnace

FY 1990
$200,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
ORNL Contact: Peter Angelini, (615) 574-4565/FTS 624-4565

This task will design and fabricate a controlled microwave furnace which can operate with a controlled atmosphere or vacuum and which is capable of operating with either 2.45 GHz or 18 GHz microwave power. In this way the optimum frequency can be used in order to process composites to improve their microstructure and properties.

Keywords: Microwave, Furnace, Frequency

53. Bulk Ceramic BiSrCaCuO and TlBaCaCuO Superconductors for Trapped-Flux Permanent Magnets

FY 1990
$350,000

DOE Contact: Marvin E. Gunn, (202) 586-5377
PNL Contact: Larry R. Pederson, (509) 375-2731
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Keywords: Superconducting Magnets, High Temperature Superconductors, HTSC

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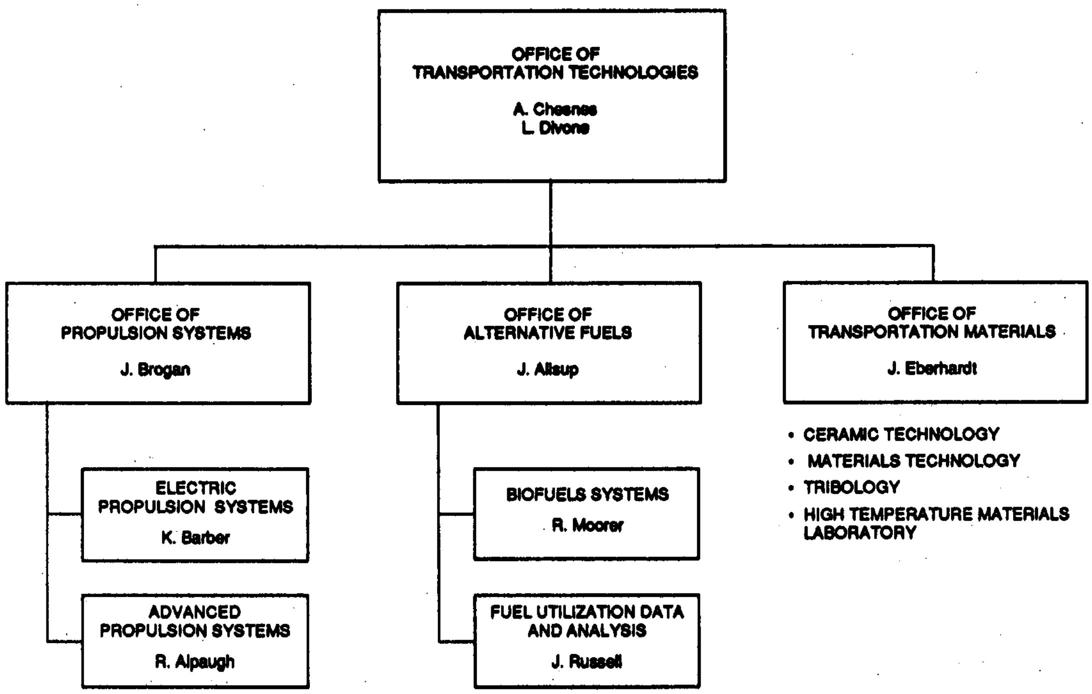
Keywords: Microwave, Furnace, Frequency

## OFFICE OF TRANSPORTATION TECHNOLOGIES

The Office of Transportation Technologies has established a number of programs to conserve energy used for transportation and to shift transportation energy demand to nonpetroleum fuels. The Office of Transportation Technologies is divided into the Office of Propulsion Systems, Office of Alternative Fuels, and Office of Transportation Materials with each having program responsibility for specific technology and program areas. The organization of the Office of Transportation Technologies is shown in the following chart.

**Organization of the Office of Transportation Technologies**




### Office of Transportation Materials

The Office of Transportation Materials conducts research programs to develop an industrial technology base in new transportation-related materials and materials processing in support of the Office of Transportation Technologies mission. Materials development activities consist of four main programmatic elements: Ceramic Technology (formerly Advanced Materials Development), Materials Technology (other than structural ceramics), Tribology, and the High Temperature Materials Laboratory.

The Ceramic Technology Program's objective is to establish an industrial technology base capable of providing reliable and cost-effective structural ceramics for applications to advanced heat engines. A balanced program is conducted in the areas of materials processing, design methodology, and data base and life prediction. A majority of the research is conducted by industry. The Ceramic Technology for Advanced Heat Engines (CTAHE) Project is managed by the Oak Ridge National Laboratory (ORNL). The DOE contact is Robert Schulz, (202) 586-8051.

The Materials Technology Program seeks to identify and resolve transportation materials problems other than those addressed under the Ceramic Technology Program. In the near-term, the program emphasizes improvements to available industry technology for materials problems in the fuel system, engine components and exhaust system of alternative-fueled (alcohol, natural gas) engines. For the mid- and long-term, the program will identify transportation-related materials requirements for electric propulsion, vehicle structure, and the transportation infrastructure. The DOE contact is James Eberhardt (Acting), (202) 586-5377.

The Tribology Program's objective is to provide a technology base for other transportation technology programs in the areas of lubrication, wear of lubricated solids, the friction and wear of ceramics, and tribological surface modifications and coatings. The Tribology Program is managed by Argonne National Laboratory (ANL). The DOE contact is James Eberhardt (Acting), (202) 586-5377.

The High Temperature Materials Laboratory (HTML) at Oak Ridge, Tennessee, is a research and user facility which supports Government and industry efforts in high temperature materials research and serves as a unique technology transfer vehicle through its user program. The HTML comprises six user centers: materials analysis, high temperature mechanical properties, high temperature x-ray diffraction, physical properties, ceramic specimen preparation, and residual stress measurements. The DOE contact is Ted Vojnovich, (202) 586-8060.

Office of Propulsion Systems

The Office of Propulsion Systems is comprised of the Advanced Propulsion Division and the Electric and Hybrid Propulsion Division. Programs supported by this office are focused on developing, in cooperation with industry through cost-shared contracts, the technologies that will lead to the production and introduction of advanced vehicle propulsion systems and electric vehicles in the nation's transportation fleet.

Advanced Propulsion Division

The Advanced Propulsion Division has two major programs: Light Duty Engine Development focused on gas turbines through the Advanced Turbine Technology Applications Project (ATTAP) and Heavy Duty Engine Development focused on diesel engines through the Heavy Duty Transport Technology (HDTT) progject. Materials activities supported by this Office and managed through the NASA Lewis Research Center for component and coating applications are included in this report. The DOE contacts are: Saunders Kramer, (202) 586-8000 for ATTAP and John Fairbanks, (202) 586-8012 for the HDTT project.

Electric and Hybrid Propulsion Division

The Electric and Hybrid Propulsion Division has three major programs: Battery Development, Fuel Cell Development, and Systems Development for electric vehicles. Materials work supported by this division is carried out by other DOE organizations and is thus not included in this section. The DOE contact is Pandit Patil, (202) 586-8055.

Office of Alternative Fuels

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

In this report, ceramic material (CTAHE) and component development (ATTAP, HDTT) projects are emphasized along with several tribology, lubricant development, and metals research projects. Not included in this report are biomass and other alternative fuel projects. Battery, fuel cell, semiconductor, electromagnetic, and other electrochemical material research that may support this office is sponsored by other DOE offices.

Materials Preparation, Synthesis, Deposition, Growth or Forming

55. High Temperature SX Carbide (WBS No. 1113) FY 1990 $381,000

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

The three major objectives for this program can be listed as follows: 1) to establish a property database and analysis for the current best SX material, 2) to optimize the processing conditions of that material using a designed experimental method, and 3) to optimize the second generation SX material with superior high temperature properties.

Keywords: High Temperature Properties, Materials Processing, Silicon Carbide

56. Turbomilling of SiC (WBS No. 1116)

FY 1990
$110,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: T. N. Tiegs, (615) 574-5173
Southern Illinois University Contact: Dale E. Wittmer, (618) 536-2396

First, a small feasibility study was conducted to investigate the use of a unique turbomilling process in the preparation of SiC whisker-toughened ceramic composites. Due to the early success of the feasibility study, the scope of this project was expanded to evaluate the effect of turbomilling variables and the beneficiation of SiC whiskers, examine the dispersion/homogenization of SiC whisker/alumina composites and SiC whisker/silicon nitride, and investigate loadings for reducing aspect ratios in the absence of coarse grinding particulate.

Keywords: Alumina, Silicon Carbide, Silicon Nitride, Turbomilling, Whiskers

57. $TiB_2$ Whiskers (WBS No. 1117)

FY 1990
$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
Keramont Contact: J. C. Withers, (602) 746-9442

The objective of this effort was to investigate the feasibility of developing a basic process to grow TiB2 whiskers by the VLS method, characterize the whisker product, and evaluate the potential of the whiskers as reinforcements for high temperature ceramic composites and metal matrix composites. Basic experimental parameters (substrate, catalyst, temperature, and gas composition) for the growth of the whiskers were defined. The whiskers produced varied in size and morphology, depending upon the experimental conditions and distance of the whiskers from the gas input port. It was concluded that while this process does have potential for scale-up, further studies would have to be performed and the process would have to be optimized to increase whisker yield and achieve growth of the whiskers in "volume" rather than on the "surface."

Keywords: Synthesis and Characterization, Testing, Titanium Diboride, Whiskers

58. Powder Characterization (WBS No. 1118)

FY 1990
$110,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. Malghan, (301) 975-2000

The objective of this effort is to develop a fundamental understanding of surface chemical changes which take place when silicon nitride powder is attrition milled in an aqueous environment.

A step-wise analysis of the underlying mechanisms controlling the material properties, and detailed characterization of the materials and their environments will be carried out. The following research is proposed:

- Characterization of the milled suspensions for physical, chemical, and surface chemical parameters to develop basic understanding of the resulting powder properties;
- An understanding of the role of milling fluids in controlling the post-milling surface chemical properties and size distribution of the powders;
- Define pertinent process variables and their influence in milling and deagglomeration;
- Develop mathematical models for simulation and control of powder production by attrition milling; and
- Evaluate resulting powders by sintering aid addition, consolidation, densification, and mechanical testing.

Keywords: Powder Characterization, Powder Processing, Silicon Nitride

59. Sintered Silicon Nitride (WBS No. 1121)

FY 1990
$145,000

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

The program is concentrating on sintering compositions in the $Si_3N_4$-$Y_2O_3$-$SiO_2$ system using a two-step sintering method where the $N_2$ gas pressure is raised to 7-8 MPa during the second step of the process. During the sintering, dissociation reactions are suppressed by the use of high nitrogen pressure and cover powder of suitable composition over the specimen.

Variables to be studied include sintering process parameters, source of starting powders, milling media and time, and specimen composition. Room temperature modulus of rupture, high temperature stress rupture, oxidation resistance, and fracture toughness have been determined.

Current efforts involve a study of "green body" forming to minimize/eliminate agglomerate formation which leads to pore development in sintered specimens. Processes such as slip casting with and without pressure will be evaluated. In addition, specimens containing the apatite phase rather than yttrium pyrosilicate should be explored with the molybdenum silicide particles distributed in the matrix.

Ceradyne, Inc., has been selected to carry out a scale-up and database generation and evaluation of a silicon nitride-yttria-silica base composition containing molybdenum carbide to be transitioned from AMTL to commercial prototype components in a turbine test engine.

Keywords: Sintering, Silicon Nitride, Testing

60. $Si_3N_4$ Powder Synthesis (WBS No. 1123) FY 1990 $ 0

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

The goal is to achieve major improvements in the quantitative understanding of how to produce sinterable $Si_3N_4$ powders having highly controlled particle size, shape, surface area, impurity content, and phase content. Of interest to the present powder needs is a silicon nitride powder of high cation and anion purity without carbon residue. The process study has been directed towards a modification of the low temperature reaction of $SiCl_4$ vapor with liquid NH3.

A pilot plant for the "vapor-chloride - liquid ammonia" direct reaction was designed and developed to pre-pilot scale. The reactor volume was increased, the quality of sealing of the vessels and piping was improved, and direct mechanical agitation to aid in by-product chloride removal was incorporated. Using this process, equiaxed, high alpha/(alpha+beta) $Si_3N_4$ was obtained. A patent, "Method of Making a High Purity Silicon Nitride Precursor," was issued, and discussions with several potential licensees are underway.

Keywords: Silicon Nitride, Synthesis and Characterization

61. Microwave Sintering (WBS No. 1124) FY 1990 $332,000

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

The objective of this effort is to identify those aspects of microwave processing of silicon nitride that might 1) accelerate densification, 2) permit sintering to high density using much lower levels of sintering aids, 3) lower the sintering temperature, or 4) produce unique microstructures.

The sintering and heat treatment of silicon nitride are being examined using a 200kW, 28 GHz furnace. Types of experiments to be performed include the following:

- Annealing of dense silicon nitride (and/or sialon) parts to examine the effects of microwave heating on grain growth and grain boundary recrystallization;
- Development of a microwave furnace dilatometer to provide the capability to monitor the densification of silicon nitride at all stages in the sintering process;
- Sintering of conventional silicon nitride compositions to establish a baseline of densification rates and microstructural states for microwave-sintered materials;
- Sintering of silicon nitride with reduced levels of sintering aids to produce a dense sintered body with superior properties at elevated temperatures; and
- Investigation of reaction-bonded (RBSN) and sintered reaction-bonded (SRBSN) silicon nitride using microwave heating.

Keywords: Microwave Sintering, Silicon Nitride

62. Novel $Si_3N_4$ Process (WBS No. 1126) FY 1990 $545,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: E. L. Long, Jr., (615) 574-5172
Sullivan Mining Corporation Contact: Thomas M. Sullivan, (619) 692-1180

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

Keywords: Materials Processing, Silicon Nitride

63. Advanced Processing (WBS No. 1141)

FY 1990
$ 0

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

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

A silicon nitride-4% yttria composition consolidated by glass encapsulated HIPing will be used. Baseline data shall be generated from an initial process route involving injection molding. Tensile test bars will be fabricated using colloidal techniques - injection molding and colloidal consolidation. Critical flaw populations will be identified using NDE and fractographic analysis. Measured tensile strength will be correlated with flaw populations and process parameters. Flaws will be minimized through innovative improvements in process methods and controls.

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

64. Improved Processing (WBS No. 1142)

FY 1990
$690,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: R. L. Beatty, (615) 574-4536

The purpose of this work is to determine and develop the reliability of selected advanced ceramic processing methods. This program is being conducted on a scale that will permit the potential for manufacturing use of candidate processes to be evaluated. An effort is being made to develop processes that can be scaled most readily to high production rates. Simplicity of processing and high predictability of product quality are dominant issues. The studies are intended to generate processing schedules and procedures as well as protocols for characterization of raw and in-process materials. The principal material of interest in this work is silicon nitride. Gel-casting, a method developed at ORNL, was the process chosen for initial consideration.

Production of tensile and other specimens of $Al_2O_3$ has demonstrated the potential for process predictability and dimensional control. A collaborative agreement with Garrett Ceramic Components Division to develop the process for silicon nitride was initiated in FY 1990.

Keywords: Alumina, Powder Processing, Silicon Nitride

65. Advanced Processing (WBS No. 1143) — FY 1990 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
GTE Contact: L. J. Bowen, (617) 466-2536

The purpose of this task is to develop the powder, process improvements, and controls needed to enable the reproducible fabrication of silicon nitride ceramics which demonstrate program goals for strength and Weibull modulus.

The material to be utilized is nominally designated PY6, a ceramic prepared from high-quality silicon nitride and yttrium oxide powders. A baseline process examined during the first year of the program will be modified using process improvements and tighter process controls which are demonstrated in parallel development activities. These improvements and controls will be incorporated into the evolving process as they are developed. Determination of the utility of any particular process improvement or process control will be made by monitoring the change in strength and Weibull modulus of uniaxial tensile specimens compared to the baseline process.

Keywords: Processing, Processing Controls, Silicon Nitride, Testing

66. Processing Science for Reliable Structural Ceramics Based on Silicon Nitride (WBS No. 1144) — FY 1990 $185,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: R. L. Beatty, (615) 574-4536
University of California, Santa Barbara, Contact: Fred F. Lange, (805) 961-8248

The objective of this effort is to obtain a basic understanding of relevant problems associated with forming powder compacts from slurries which will densify to produce reliable structural ceramics.

The overall approach of this research is to obtain fundamental relations between slurry rheology, particle packing mechanics, consolidated body rheology, strain recovery, and powder compact integrity. It is expected that this understanding will lead to a definition of the colloidal and rheological requirements to reliably process advanced ceramics with improved property reliability and to new slurry consolidation methods.

Keywords: Powder Processing

67. Dispersion Toughened $Si_3N_4$ (WBS No. 1221) FY 1990 $532,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Garrett Ceramic Components Division Contact: H. C. Yeh, (213) 618-7449

For Phase I, the approach was to develop a silicon nitride matrix composite with SiC whiskers dispersed in the matrix using standard powder processing specifications in place at Garrett, and sintering and/or HIPing for final consolidation. Elastic modulus, four-point bend strength, density, thermal expansion, thermal conductivity, and fracture toughness were determined. In addition, a low cost, near-net-shape process was developed.

The objective of Phase II of this program is to maximize the toughness in a high strength, high temperature SiC whisker/$Si_3N_4$ matrix material system that can be formed to shape by slip casting and densified by a method amenable to complex shape mass production. The ASEA glass encapsulation hot isostatic pressing (HIP) technique shall be used for densification throughout the program. Following selection of a SiC whisker as the reinforcement in GN-10 $Si_3N_4$ matrix, process optimization and property evaluation studies will commence.

Keywords: Silicon Carbide, Composites, Silicon Nitride, Sintering, Hot Isostatic Pressing, Whiskers, Testing, Physical/Mechanical Properties

68. Dispersion Toughened $Si_3N_4$ (WBS No. 1223) FY 1990 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
GTE Contact: S. T. Buljan, (617) 890-8460

For Phase I, the approach was to closely examine toughening of $Si_3N_4$ through introduction of refractory, particulate, or whisker dispersoids. The initial phase development was based on a commercial $Si_3N_4$ material, GTE AY6, and additions of SiC and TiC whisker or particulate dispersoids. For the purposes of screening, the composites were densified by hot pressing. Mechanical and physical properties of consolidated composites were then evaluated and their microstructure thoroughly examined in order to define property-microstructure relationships and establish design parameters for further material modification. The most promising candidate developed in Phase I would serve as a basis for development of the near-net-shape fabrication process.

During Phase II, silicon nitride powders and whiskers from several sources were evaluated as raw materials for composite fabrication. Concurrent studies on the effects of sintering aids on microstructure development and properties demonstrated that composition of the intergranular phase plays a deciding role in the toughening of $Si_3N_4$. Modifications of material and process parameters have resulted in additional improvement of composite fracture toughness. Utilization of the crack deflection mechanism was found effective in producing composites of nearly twice the fracute toughness of the starting monolith with concomitant increases in both room and elevated temperature strength. Focusing on dimensional control, the process for near-net-part fabrication by injection molding was further improved. Properties of near-net-shape parts equaled those obtained on hot pressed laboratory specimens. The developed technology has been transferred and incorporated into ATTAP where it was utilized in injection molding of the ATTAP rotor.

Keywords: Silicon Nitride, Composites, Sintering, Whiskers, Physical/Mechanical Properties

69. <u>Composite Development (WBS No. 1224)</u> — <u>FY 1990</u> $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: P. F. Becher, (615) 574-5157
Norton Contact: N. D. Corbin, (508) 393-5829

The objective of Phase I of this task was the development of fully dense $Si_3N_4$ matrix SiC whisker composites with enhanced properties over monolithic $Si_3N_4$ materials. The emphasis of this study was on utilizing the (Hot Isostatic Pressure) HIP process which has the potential for producing near-net-shaped complex geometries. The primary goal was to develop a composite with a fracture toughness of >10 MPa and capable of operating up to 1400 °C.

Coating methods were developed to apply thin stoichiometric BN layers to SiC whiskers and also to apply a dual coating of SiC over carbon to the whiskers. Fracture toughness of the composites was found to increase as the quantity of whiskers (or elongated grains) with their axises perpendicular to the crack plane increased. Of the interface compositions evaluated as part of this effort, carbon was determined to be the most effective for increasing toughness. Highest toughnesses were obtained with uniaxially aligned carbon-coated whiskers. There was no evidence of the carbon coating compromising oxidation resistance of the composites at 1370 °C.

Keywords: Composites, Silicon Carbide, Silicon Nitride, Hot Isostatic Pressing, Sintering, Fracture Toughness

70. Advanced Composites (WBS No. 1225) FY 1990
$205,000

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

The goal of this project is to obtain dense silicon nitride composites containing silicon carbide whiskers by transient liquid phase sintering. The systems SiAlON, SiAlON-Garnet ($Y_3Al_5O_{12}$) and SiAlON-Cordierite ($Mg_2Al_4Si_5O_{18}$) were selected for this study. Mixtures of the starting materials form a sufficient amount of liquid to aid densification at the sintering temperatures. After sintering, the liquid can be crystallized by heat treatment.

Keywords: Composites, Silicon Nitride, Silicon Carbide, Sintering, SiAlON

71. Dispersion Toughened Oxide Composites (WBS No. 1231) FY 1990
$360,000

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

This work involves development and characterization of SiC whisker-reinforced oxide composites for improved mechanical performance. Although most of the early work dealt with alumina as the matrix, efforts in SiC whisker reinforced-SiAlON-based materials and silicon nitride have been initiated. Whisker synthesis was examined to develop whiskers with high strength which would enable high toughness composites to be produced. In addition, a study to develop high toughness silicon nitride materials by growth of elongated grain microstructures was initiated.

Keywords: Composites, Alumina, Silicon Carbide, SiAlON

72. Transformation Toughened Ceramics Processing (WBS No. 1232) FY 1990
$128,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Norton Contact: Giulio A. Rossi, (508) 393-6600

During Phase I, emphasis was on production of improved zirconia toughened ceramics for advanced engine applications. The scope included powder synthesis and characterization of the sintered ceramics. Materials made from three powder sources were evaluated: a rapid solidification from-the-melt powder, and two chemically-derived powders. Rapidly solidified powders showed better performance than chemically-derived powders.

For Phase IIA of this program, the main effort for the Y-TZP materials has been to study the low-temperature degradation and understand how it is affected by microstructure and composition. Major improvements have been made by means of chemical uniformity, higher yttria, and finer grain sizes. In the case of the Ce-ZTA ceramics, the main goal was to optimize the mechanical properties. The pressureless sintered Ce-ZTA composites made with a R/S powder by colloidal consolidation have shown excellent microstructures and mechanical properties, with good property retention at high temperature. The Ce-ZTA composites are believed to be excellent candidates for heat engine applications.

Keywords: Composites, Zirconia, Sintering, Alumina, Synthesis and Characterization

73. <u>Development of Toughened Ceramics (WBS No. 1237)</u> <u>FY 1990</u> $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Ceramatec Contact: R. A. Cutler, (801) 486-5071

Phase I of this project involved the development of layered ceramic composites which incorporate zirconia as a second phase to achieve improved strength and toughness at temperatures of up to 1000°C. The work also addressed processing methods for fabricating these layered composites via sintering.

Results from Phase I have shown that it is possible to increase the strength of $Al_2O_3$-$ZrO_2$ ceramics by incorporating transformation-induced residual stresses in sintered specimens consisting of three layers.

Phase II objectives included: 1) increasing the use temperature of three-layer composites by substituting $HfO_2$ for $ZrO_2$; 2) developing aqueous and nonaqueous slip casting techniques for three-layer composites in order to obtain better layer uniformity and to maximize residual compressive stress by optimizing the outer layer thickness; 3) superimposing temperature stresses on transformation-induced stresses in three-layer composites; and 4) demonstrating improved thermal shock resistance and damage resistance in optimized composites.

Ceramatec has developed layered DTA composites which incorporate zirconia or hafnia as a second phase to achieve improved strength and toughness at temperatures of up to 1000°C. Slip casting methods were developed to produce three-layer composites with room temperature strengths in excess of 1200 MPa, and 600 MPa at 1000°C.

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

74. Low Expansion Ceramics (WBS No. 1242) FY 1990
$253,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: Victor J. Tennery, (615) 574-5123
Virginia Polytechnic Institute and State University Contact: J. J. Brown, (703) 961-6640

A major objective of this research is to investigate selected oxide systems for the development of a low expansion, high thermal shock resistant ceramic. Specifically, it is the goal of this study to develop an isotropic, ultra-low thermal expansion ceramic which can be used above 1200°C and which is relatively inexpensive, and to determine conditions necessary for synthesis, densification, and characterization of these systems.

The research program includes synthesis, property characterization, and fabrication of candidate low thermal expansion ceramics from four systems based on beta-eucryptite, silica, mullite, and zircon. At the present time, encouraging results have been obtained for the development of improved thermal shock resistant beta-eucryptite and zircon (NZP) compositions.

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

75. Vapor-Phase Lubrication System FY 1990
$75,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
The Pennsylvania State University (NIST Grant No. 60NANB5DO548) Contact: E. E. Klaus, (814) 865-2574

The objective of this project is to develop a novel, vapor-phase lubrication system for advanced heat engines. A system has been developed to deliver the vapor-phase lubricants to surfaces and produce a lubricating film. Initial feasibility was demonstrated in the four-ball tester. The current study expands the lubrication research to ceramics using the ball-on-three-flats configuration. The lubrication types to be evaluated in the wear tester will include those that show reaction and deposition on ceramic specimens at high-temperatures in static tests. High-temperature friction and wear studies will be conducted at NIST.

Deposition-rate studies and the identification of the chemical mechanisms involved will be continued using SiC, $Si_3N_4$ and $Al_2O_3$ as the substrates. Compounds in the 200-600 molecular-weight range that contain various polar functional groups will be evaluated. The rates of interaction will be determined.

At temperatures exceeding about 500°C (such as in low heat rejection engines), it is not practical to consider liquid-lubrication modes due to rapid deposit formation, thermal and oxidative decomposition of organic and metallic-organic molecules. By selection of the proper compounds, and reducing the concentration of these compounds exposed to the hot surfaces, control of deposits and friction and wear are feasible and have been demonstrated by PSU. The method has also been successfully tested in an experimental engine cylinder kit by Detroit Diesel Allison Division of G.M.

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

76. Ion-Beam-Assisted Deposition of Lubricious Compounds — FY 1990 $200,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
ANL (Contract No. W-31-109-ENG-38) Contact: Fred Nichols, (312) 972-8292

This activity focuses on the development of ion-beam-assisted deposition (IBAD) processes for low-friction coatings on engineering surfaces. It involves efforts to develop IBAD processes, to characterize IBAD-deposited films by electron microscopy and mechanical-testing techniques, and to evaluate their tribological performance under different conditions. Past process development focused on the design and construction of IBAD facilities. The design and construction phase is nearly completed with minor modifications being made to improve turn-around time, improve the base pressure in the chamber, and to provide the ability to deposit coatings with reactive ions. The majority of the current effort is now focusing on the preparation of samples for subsequent characterization and wear testing. During FY 1990, design modifications formulated during FY 1989 will be implemented to provide the ability to generate IBAD coatings in a reactive environment on components with complex shapes.

Keywords: Ion-Beam-Assisted Deposition, Coatings, Tribology, Friction, Wear

77. Ion Implantation/Mixing of Lubricious Oxides — FY 1990 $60,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
ANL (Contract No. W-31-109-ENG-38) Contact: Fred Nichols, (312) 972-8292

The objective of this effort is to assess the feasibility of forming a lubricious compound ($B_2O_3$) of boron in near-surface regions of high-temperature metallic alloys and ceramics by ion implantation of B or ion-beam mixing of B and Fe layers. A series of substrates (hardened bearing steels, superalloys, and $Al_2O_3$) will be implanted with B ions and subjected to a series of friction and wear tests at different temperatures and loads to determine if a lubricious compound forms as evidenced by a decrease in the coefficient of friction. In another series of experiments, multiple layers of Fe and B (or $B_2O_3$) will be deposited by PVD techniques and subsequently ion-beam-mixed. These coated samples will then be subjected to a series of friction and wear tests similar to the ion-implanted samples to determine if the frictional properties are improved.

During FY 1990, this effort will start to focus on ion-beam mixing of Fe/B (or Ti/B) coatings deposited on steel and ceramic substrates. The research will emphasize high-temperature friction and wear testing in contrast to the room-temperature testing performed thus far in the program. The ion implantation will focus on high-dose and/or lower-energy implantations of B. This is due to the need to increase the concentration of B in the near-surface regions. The implantations studied thus far used 160-keV B ions at doses of $10^{21}$ m-2, resulting in near-surface B concentrations of approximately 10-20 percent. The new implantations at 40 to 60 keV to doses of 2 x $10^{21}$ $m^{-2}$ should result in significantly higher concentrations of B on the surface thus providing a reservoir of B to form lubricious B compounds.

Keywords: Ion Implantation, Ion-Beam Mixing, Coatings, Tribology, Friction, Wear

78. HRRS Hard Coatings — FY 1990 $90,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
BIRL Contact: Raymond Fessler, (708) 491-4941

The high-rate reactive-sputtering process showed great promise for producing well-adherent, hard, wear-resistant coatings on steel substrates. Significant increases in the cutting lifetimes of coated inserts were observed; however, the wear mechanisms and in particular the effects of frictional heating on the coating failure are not fully understood. During FY 1990, a research effort was initiated with the Basic Industry Research Lab (BIRL) to deposit nitride and carbide coatings of Ti, Zr and Hf on steel and ceramic substrates. These samples are subjected to rolling-contact fatigue and oscillating-wear tests to provide information on the friction, wear and fatigue properties. In future years, the effort will investigate the role of small additions of As, Sb and Bi in increasing the hardness of the coatings.

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

79. Additives for High-Temperature Liquid Lubricants — FY 1990 $ 0

DOE Contact: J. J. Eberhardt, (202) 586-1694
JPL Contact: Emil Lawton, (818) 354-2982

Additives currently available are generally designed to be effective and perform well at temperatures well below 200°C, lower than those encountered in low heat rejection engines. Volatility as well as both thermal and oxidative stability are some of the areas requiring improvement. Dinitrile compounds are in one chemical family that possesses the potential to meet some of the desired properties.

The basic thrust of this activity will be to synthesize at least six precursor dinitrile compounds to be evaluated as lubricant additives. These compounds may react *in situ* with the sliding contact surfaces forming lubricating films. The compounds will be selected so that information on the effect of chemical structure on high-temperature properties can be determined.

The compatibility of the proposed compounds with ceramic surfaces and lubricant additives that are commonly used in lubricating oils will be determined. The physical properties, and thermal and oxidative stability of these compounds will also be determined. The effect of molecular structure, as well as the mechanism of action of these molecules will be investigated.

Results of the initial work will be directed toward synthesis of more promising additive compounds. The expected outcomes of this research are effective lubricant additives produced in large quantities for subsequent testing and characterization, and verification of the lubrication mechanism(s) to be used as a guide for future additive development.

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

80. IBAD of TiN and $Cr_2O_3$ FY 1990
$75,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
NRL (Contract No. DE-AI02-88CE90024) Contact: Fred Smidt, (202) 767-4800

The objective of this project is to determine the mechanism by which ion-beam-assisted deposition (IBAD) produces beneficial modifications of tribological coatings and to establish the necessary correlations between processing parameters and microstructural features of the coating and tribological properties such as friction, wear, and adhesion. General principles for producing the improved coatings will then be defined for the application of these coatings to advanced energy systems.

During FY 1990 the work on IBAD TiN films focused on depositing a series of thick (2.0 to 5.0 $\mu$m) coatings on steel or silicon substrates. Direct comparisons were made to HRRS coatings in terms of friction, wear life in dry sliding and adhesion as determined by an acoustic-emission scratch tester. Fracture surfaces were produced for examination of coating cross-sections using high-resolution SEM to determine structure (i.e., columnar, equiaxed, etc.) as a function of deposition parameters. Chromium oxide films were also deposited by IBAD using argon- or oxygen-ion bombardment coincident with Cr evaporation in an oxygen-gas backfill. Several correlations of film properties (adhesion, microhardness, and friction coefficient) with processing parameters will be established.

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

81. Self-Lubricating Ceramic Surfaces

FY 1990
$75,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
Universal Energy Systems (Contract No. DE-AC02-88CE900026) Contact: Rabi Bhattacharya, (513) 426-6900

This project seeks to establish optimal conditions for ion implantation and ion-beam mixing of suitable additives into the surfaces of bulk $ZrO_2$, $Al_2O_3$ and hardened steel for obtaining self-lubricating low friction and wear characteristics. A series of $Al_2O_3$, $ZrO_2$ and steel substrates will be co-implanted with $Mo^+$ and $S^+$, $Ta^+$ and $S^+$ and subsequently annealed to form $MoS_2$ and $TaS_2$ respectively. In another series of experiments, multiple layers of $BaF_2/CaF_2/Ag$ will be deposited and subsequently ion-mixed at elevated temperatures. After appropriate characterization using SEM, TEM, and RBS techniques and optimization of the mixing process, samples will be prepared for friction and wear tests. Initially, ion implantation and subsequent annealing are being performed to synthesize these additives in the near-surface region. Ion beam mixing of thin films of these additives at room temperature and elevated temperature will be investigated and results will be compared with that of direct ion implantation.

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

Materials Properties, Behavior, Characterization or Testing

82. Microstructural Modeling of Cracks (WBS No. 2111)

FY 1990
$82,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
University of Tennessee Contact: J. A. M. Boulet, (615) 974-2171

A goal of this research is to develop mathematical procedures by which existing design methodology for brittle fracture could accurately account for the influence of non-planar crack faces on fracture of cracks with realistic geometry under arbitrary stress states. Existing models all consider the crack faces to be smooth and planar, but examination of fresh fracture surfaces by microscopy often indicates rough, irregular surfaces. In this study, the effect of protrusion interference on fracture of cracks with realistic geometry under arbitrary stress states is being examined.

Keywords: Predictive Behavior Modeling, Structural Ceramics

83. Adherence of Coatings (WBS No. 2212)

FY 1990
$22,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: C. J. McHargue, (615) 574-4344

Financial support is provided for a graduate research assistantship in the Department of Materials Science and Engineering at the University of Tennessee to conduct studies on adherence of coatings deposited on substrates subjected to ion beam mixing.

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

84. Dynamic Interfaces (WBS No. 2221)

FY 1990
$109,000

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

The objective of this study is to develop an understanding of the friction and wear processes of ceramic interfaces based on experimental data. The supporting experiments are conducted at temperatures to 650 °C under reciprocating sliding conditions reproducing the loads, speeds, and environment of the ring/cylinder interface of advanced internal combustion engines. The test specimens are carefully characterized before and after testing to provide detailed input into the model.

Current efforts are addressing the performance of advanced toughened monolithic ceramics, thermal-spray coatings, surface modifications, and high temperature lubricants. The test rig developed in this program has been shown to give results similar to actual engine tests by the major diesel engine producers, but the rig tests are much quicker and cheaper.

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

85. Advanced Statistics Calculations (WBS No. 2313)

FY 1990
$ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
GE Contact: C. A. Johnson, (518) 387-6421

The design and application of reliable load-bearing structural components from ceramic materials requires a detailed understanding of the statistical nature of fracture in brittle materials. The overall objective is to advance the current understanding of fracture statistics, especially in the following areas:

- Optimum testing plans and data analysis techniques;
- Consequences of time-dependent crack growth on the evolution of initial flaw distributions; and
- Confidence and tolerance bounds on predictions that use the Weibull distribution and function.

The studies are being carried out largely by analytical and computer simulation techniques. Actual fracture data are then used as appropriate to confirm and demonstrate the resulting data analysis techniques.

Keywords: Design Codes, Life Prediction, Statistics, Weibull, Fracture, Structural Ceramics, Instrumentation or Technique Development

86. Microstructural Analysis (WBS No. 3111) FY 1990
$50,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. M. Wiederhorn, (301) 975-2000

The objective of this work is to identify the mechanisms of failure in structural ceramics subjected to mechanical loads in various test temperatures and environments. This is a companion project to a related task in which advanced ceramics are characterized in tensile creep. Scanning and transmission electron microscopy are used to characterize damage accumulation in the creep specimens.

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

87. Microstructural Characterization of Silicon Carbide and Silicon Nitride Ceramics for Advanced Heat Engines (WBS No. 3114) FY 1990
$205,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: T. A. Nolan, (615) 574-0811

The purpose of this work is to determine the microstructure of both monolithic and composite ceramics and to relate that microstructure to mechanical properties and material performance. Specifically, the materials of interest are silicon carbides and silicon nitrides developed by U.S. manufacturers as part of this program and the ATTAP. A major objective is to use electron microscopy and surface chemistry to characterize the chemistry, crystallography, and morphology of phases present with particular emphasis on the structure and chemistry of grain boundaries and other interfaces.

A second major objective is to relate those microstructural observations to available mechanical test data produced by other participants in the ATTAP and Ceramic Technology programs. Ceramic specimens from foreign sources are also characterized to provide comparative information on microstructural properties.

Keywords: Silicon Carbide, Silicon Nitride, Microstructure, Chemical Analysis, Mechanical Properties

88. Project Data Base (WBS No. 3117) — FY 1990 $105,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: B. L. Keyes, (615) 574-5113

This task involves efforts to develop and maintain a computer data base of mechanical property data generated in the Ceramic Technology for Advanced Heat Engines program. The data base system is currently composed of a loosely-connected framework of commercially available programs. However, data can be easily transferred by electronic means to a variety of other programs. Techniques have been developed that allow data as compiled on a variety of computers using several different software programs to be transferred directly into the data base electronically with no manual transcription of the data. Several techniques for data output in useful formats (tabular and graphical) have also been developed. The system has been designed to provide maximum flexibility to allow the addition of other data as the data base grows.

Reports containing mechanical properties and material characterization information on silicon nitride, silicon carbide, zirconia-based, and transformation-toughened ceramics as well as test data files on brazed specimen torsion strength and torsion fatigue have been issued.

Keywords: Database, Mechanical Properties, Structural Ceramics

89. Characterization of Transformation-Toughened Ceramics (WBS No. 3211)

FY 1990
$100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
AMTL Contact: Jeffrey J. Swab, (617) 923-5410

The main objective is to determine the effect of time-at-temperature on transformation toughened zirconias, especially tetragonal zirconia polycrystals (TZP) at engine operating temperatures (1000-1200 °C). A preliminary study of the degradation of mechanical properties at low temperatures (200-400 °C) in yttria-doped zirconias has also been initiated.

Due to the inherent problems of TZPs at low and high temperatures, evaluation and characterization of these materials are currently being phased out. The next generation of promising materials, composite ceramics toughened by fibers, whiskers, or particulates, will be studied instead. Following an initial screening, selected composite ceramics will be evaluated in detail using a similar evaluation matrix.

Keywords: Alumina, Transformation Toughened Zirconia, High Temperature Service, Engines, Fracture, Mechanical Properties

90. Fracture Behavior of Toughened Ceramics (WBS No. 3213)

FY 1990
$290,000

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

Analytical modeling and experimental studies have been aimed at providing fundamental insights into the processes responsible for toughness and time-dependent strength degradation of materials such as silicon carbide, silicon nitride, partially-stabilized zirconia, and dispersion-toughened and whisker-reinforced oxides. Particular emphasis is being given to understanding the effect of environment, temperature, and compositional and microstructural characteristics upon these mechanisms. In addition, fundamental insight into the slow crack growth behavior associated with these materials is being obtained.

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

91. Cyclic Fatigue of Toughened Ceramics (WBS No. 3214)

FY 1990
$286,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: K. C. Liu, (615) 574-5116

Using the special tensile testing system designed, fabricated, and tested at ORNL, elevated temperature tensile and fatigue tests are being performed on candidate monolithic ceramic materials such as silicon nitride. Exploratory creep tests were performed on an advanced silicon nitride at elevated temperatures above 1200 °C. Constant loads were applied uniaxially to buttonhead tensile specimens, and creep strain was measured using an optical strain extensometer. Test results indicated that the creep behavior of virgin specimens is reasonably consistent within the same lot and, therefore, predictable. However, lot-to-lot variations in creep deformation preclude a simple mathematical representation for the time-dependent behavior.

In addition, several specimens were precycled in a tension/tension mode to a peak stress of about 220 MPa for a period of 150 h prior to testing in creep at 1300 and 1370 °C. Results from this limited testing showed that the precyled specimens exhibited strain recovery immediately following initial loading, in dramatic contrast to the pronounced primary creep behavior seen in the virgin specimens. It appeared that the distinctive behavior changes were due to microstructural changes occurring during the precycling.

Keywords: Cyclic Fatigue, Toughened Ceramics, Tensile Testing, Silicon Nitride

92. Tensile Stress Rupture Development (WBS No. 3215)

FY 1990
$321,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: K. C. Liu, (615) 574-5116

The objective of this task is to develop the test capability for performing uniaxial tensile stress-rupture tests on candidate structural ceramics. Existing data requirements specify that tensile creep-rupture data be developed in the range of 1260 °C to 1371 °C. These data bases are to be generated using cylindrical bar specimens of materials such as silicon nitride with the tests conducted in an air environment. Ten standard uniaxial level arm creep frames were modified to incorporate the specimen load train with a self-aligning feature and closed-loop control capability. Proper design of the furnace to produce a uniform temperature zone at the required temperature while minimizing specimen grip temperature was mandatory. A laser interference fringe technique is employed for creep measurements.

Keywords: Silicon Nitride, Tensile Testing

93. Rotor Materials Data Base (WBS No. 3216) FY 1990 $315,000

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

The goal of this research program is to systematically study the tensile strength of a silicon nitride and a silicon carbide ceramic as a function of temperature and time in an air environment. Initial tests were aimed at measuring the statistical parameters characterizing the strength distribution of three sample types. The resulting data will then be used to examine the applicability of current statistical models as well as sample geometries for determining the strength distribution.

Next, stress rupture data will be generated by measuring fatigue life at a constant stress. The time-dependent deformation will also be monitored during testing so that the extent of high-temperature creep may be ascertained. Tested samples will be thoroughly characterized using established ceramographic, SEM, and TEM techniques. A major goal of this effort will be to better understand the microstructural aspects of high-temperature failure.

The resulting stress rupture data will be used to examine the applicability of a generalized fatigue-life (slow crack growth) model. If necessary, model refinements will be implemented to account for both crack blunting and creep damage effects. Once a satisfactory model is developed, separate stress-rupture (confirmatory) experiments will be performed to examine the model's predictive capability.

Keywords: Creep, Engines, High Temperature Service, Structural Ceramics, Tensile Testing, Predictive Behavior Modeling

94. Toughened Ceramics Life Prediction (WBS No. 3217) FY 1990 $327,000

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

The objective of this effort is to determine the behavior of toughened ceramics, especially SiC whisker-toughened $Si_3N_4$, as a function of time and temperature as the basis for developing a life prediction methodology. The room temperature and elevated temperature strength and reliability, the fracture toughness, slow crack growth, and the creep behavior will be determined for the as-manufactured material. The same properties will be evaluated after long-time exposure to various high temperature isothermal and cyclic environments.

A second major effort will be to better understand the relationship between microstructure and mechanical behavior for a limited number of materials. These results will provide input for parallel materials development and design methodology development. Resultant design codes will be verified.

Keywords: Creep, Fracture Toughness, Life Prediction, Silicon Nitride

95. Ceramic Durability Evaluation AGT — FY 1990 $80,000

DOE Contact: Saunders B. Kramer, (202) 586-8000
NASA Contact: Sunil Dutta, (216) 433-3282
Garrett Turbine Engine Contact: Nancy Campbell, (602) 220-7006

The objective of the program is to evaluate commercially available structural and glass ceramic material specimens exposed to combustion products at temperatures up to 2500 °F for periods up to 3,500 hours. In 1989, Kyocera SN-251 silicon nitride and Carborundum $TiB_2$ and silicon carbide were tested.

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

96. Environmental Effects in Toughened Ceramics (WBS No. 3314) — FY 1990 $109,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: Victor J. Tennery, (615) 574-5123
University of Dayton Contact: N. L. Hecht, (513) 229-4341

The objective of this task is to characterize the mechanical behavior and environmental degradation processes operative in candidate AGT ceramics using flexural and uniaxial tensile testing and extensive pre- and post-test characterization of physical properties and microstructure.

Flexural strength is being measured over a wide range of stressing rates, temperatures, and atmospheric conditions to quantitatively determine relevant fatigue parameters.

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

97. LHR Diesel Coupon Tests (WBS No. 3315) — FY 1990 $150,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: C. R. Brinkman, (615) 574-5106

The objective of this effort is to subject a number of candidate advanced ceramic materials and metal-ceramic joints to low heat rejection (LHR) diesel engine environments where the effects of a number of variables (e.g., temperature, fuel type, and engine operating conditions) can be determined.

Following characterization (i.e., dimensions, weight, density, and a quality assurance inspection for defects), small rectangular test bars of candidate ceramic material are inserted into a single-cylinder diesel engine combustion chamber. Engine insertion periods typically average up to 1000 hours. After exposure, the specimens are removed and examined for four-point bend rupture testing and the results compared to the unexposed material database. Engine operating conditions are varied to impose thermal transients, and specimen temperatures are monitored.

Keywords: Diesel Engines, Structural Ceramics, Testing

98. High Temperature Tensile Testing (WBS No. 3412) — FY 1990 $218,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
North Carolina A&T State University Contact: V. Sarma Avva, (919) 334-7620

The objective of this task is to test and evaluate advanced ceramic materials at temperatures up to 1500 °C in uniaxial tension. Testing may include fast fracture strengths and stepped static fatigue strength along with analysis of fracture surfaces by scanning electron microscopy.

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

99. Standard Tensile Test Development (WBS No. 3413) FY 1990 $125,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. M. Wiederhorn, (301) 975-2000

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

Two inexpensive techniques for tensile testing have been developed at NIST. These techniques are being used to test materials intended for heat engines. The results obtained by high temperature tensile testing will be compared with those obtained by compressive and flexural testing. Data obtained from these studies will be compared with various theories of creep and creep rupture that have been developed to date. Based on the data obtained from these studies, a methodology for high temperature design will be recommended.

Keywords: Creep, Structural Ceramics, Tensile Testing

100. Development of a Fracture Toughness Microprobe (WBS No. 3415) FY 1990 $72,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: W. C. Oliver, (615) 576-7245
Rice University Contact: G. M. Pharr

The objective of this effort is to develop a technique for measuring fracture toughness in thin films and small volumes on a spatially-resolved basis. The Mechanical Properties Microprobe will be used to develop the technique.

Keywords: Fracture Toughness, Structural Ceramics, Testing

101. Non-Destructive Evaluation (WBS No. 3511) FY 1990 $360,000

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

The purpose of this program is to develop nondestructive evaluation (NDE) techniques in order to identify approaches for quantitative determination of conditions in ceramics that affect the structural performance. High-frequency ultrasonics and radiography are being used to detect, size, and locate critical flaws and to nondestructively measure the elastic properties of the host material.

Keywords: NDE, Radiography, Structural Ceramics, Ultrasonics

102. Computed Tomography (WBS No. 3515) FY 1990
$65,000

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

The objectives of this program are to: 1) develop necessary techniques for reliable use of polychromatic X-ray computed tomography to characterize structural ceramics relative to density distributions, presence of voids, inclusions, and cracks; and 2) develop calibration methods for CT scanners for ceramic materials.

Argonne is using 1) an available medical CT scanner which has had extensive software modifications for ceramic applications; 2) commercially prepared ceramics ($Si_3N_4$, SiC, $Al_2O_3$, and $ZrO_2$), and compounds tailored for specific mass and electron density; and 3) available international attenuation coefficient tables. There are two distinct parts to the approach: 1) development of a calibration phantom, and 2) corrections for streak artifacts.

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

103. Nuclear Magnetic Resonance Imaging (WBS No. 3516) FY 1990
$136,000

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

The objectives of this program are to 1) establish the feasibility of using NMR imaging systems to map organic B/P distributions in injection-molded green ceramics, 2) examine the potential for NMR spectroscopy to determine if there are any chemical variations within and/or between batches of organic binder which impact process reliability, and 3) determine the sensitivity of NMR imaging methods to injection molding process variables as manifested in distribution of the organic.

Argonne has demonstrated that NMR imaging with appropriate techniques, field gradient strength, and with correct back projection imaging algorithms, polymeric binders can be imaged at room temperature. In addition, with appropriate filler fluids, NMR imaging can be used to detect defects in partially densified ceramics. A 2-T superconducting-magnet NMR imaging system has been used to evaluate the feasibility of imaging B/P directly. Green state test specimens were made by mixing various wt. % binder with $Si_3N_4$ powder.

Keywords: Binder, Nuclear Magnetic Resonance, Silicon Nitride

104. Powder Characterization (WBS No. 3517) — FY 1990 $100,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
ORNL Contact: O. O. Omatete, (615) 576-7199

Objectives for this effort include: 1) identification, characterization, and modification of those aspects of the chemistry and physics of a ceramic powder and of the powder/solvent interface that control processing; 2) development of standard methods of analysis for achieving (1), and 3) development of procedures for writing specifications for ceramic powders that include any of the methods of analysis developed during this project.

The approach is a combination of basic science and applied engineering. ORNL and three universities are participating in the project. There are three distinct elements:

- A round-robin characterization of electrophoretic mobility and acid-base character in aqueous suspension to be conducted by all participants.

- Gas chromatography of $Si_3N_4$ surfaces and electrophoretic studies of slurries for gel casting to be performed by ORNL, and special projects to be performed at each university which are described in project summaries for WBS Nos. 3518, 3519, and 3520.

- Adaptation and verification of analytical procedures developed during the project to determine their usefulness in the research laboratory or in industrial practice.

Keywords: Powder Characterization

105. Spectroscopic Characterization (WBS No. 3518)

FY 1990
$76,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
University of Wisconsin Contact: M. A. Anderson, (608) 202-2470

This is one of three companion tasks to develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics. The objective of this particular effort is to perform a thorough spectroscopic analysis and characterization of selected ceramic powders and/or whiskers in non-aqueous suspension. The spectroscopic studies will be supported by other surfaces studies such as adsorption isotherm determination, calorimetry, and light scattering, etc., to confirm and amplify the data generated in the spectroscopic studies.

Keywords: Powder Characterization, Spectroscopy

106. Surface Adsorption (WBS No. 3519)

FY 1990
$138,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
Pennsylvania State University Contact: J. H. Adair, (814) 863-0857

This is one of three companion tasks to develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics. The purpose of this effort is to conduct a study of the basic mechanisms of adsorption from non-aqueous solvents onto ceramic surfaces, and the modification of those surfaces to make them uniformly processable. Adsorption studies on both monomers and polymers will be considered. Various gas-phase treatments that might be applied to the ceramic powders to make their surfaces more uniform may also be pursued.

Keywords: Powder Characterization, Surface Modification

107. Thermodynamics of Surfaces (WBS No. 3520) FY 1990 $82,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. A. Janney, (615) 574-4281
Rutgers University Contact: D. J. Shanefield, (201) 932-2226

This is one of three companion tasks to develop an understanding of the critical characterization parameters for powders to be used as the starting materials for high-performance ceramics. The objective of this task is to determine the thermodynamic nature of the ceramic powder surface in non-aqueous powder suspension. The methods take the form of the Drago analysis for non-aqueous solvents or may use some other formalism such as that used in chromatographic studies. The result that one may reasonably expect from such a study is a set of classification categories for ceramic powders, binders, dispersants, etc., that will guide ceramic process engineers in their selection of processing aids for a particular ceramic powder.

Keywords: Powder Characterization, Thermodynamics

108. Effect of a Lubricating Surface Layer on the Wear Mechanisms in Silicon Carbide-Whisker-Reinforced Silicon Nitride FY 1990 $130,000

DOE Contact: J.J. Eberhardt, (202) 586-1694
ORNL (Contract No. DE-AC05-840R21400) Contact: Peter Blau, (615) 574-1514

It is well recognized that ceramics in many proposed high-temperature applications will require lubrication to function effectively. The importance of liquid-lubrication effects in $Al_2O_3$ matrix, SiC-whisker-reinforced composites has been determined. This investigation will be extended to $Si_3N_4$ matrix materials. Efforts will be devoted to solid lubrication for higher-temperature, sliding-contact environments. Studies of the subsurface damage mechanisms and the deformation-induced fracture of the composite during wear will be conducted. Furthermore, observations on the wear-debris layers formed on solid-lubricated contacts may be used in developing a new third-body wear model.

Friction and wear of ceramics at elevated temperature is of particular interest since this is the temperature range in which the use of ceramics is most advantageous. Previous results at ORNL for unlubricated sliding of $Al_2O_3$-SiC and zirconia-toughened composites at a temperature over 400 °C indicated that severe friction and wear occur at applied normal forces of 2 to 8 N. Further tests showed, however, that the zirconia-toughened matrix material alone did not exhibit the same wear behavior. X-ray diffraction studies then led to the discovery that the relative amounts of tetragonal and monoclinic phases in the zirconia particles in the composite and in the matrix alone were different. Crystallographic modification of the zirconia particles by altering the heat treatment subsequently began in FY 1990 to improve the wear of the composite over 400 °C.

Keywords: Solid Lubrication, Ceramic Composites

109. IBAD Process Characterization

FY 1990
$250,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
ANL (Contract No. W-31-109-ENG-38) Contact: Fred Nichols, (312) 972-8292

The objective of the process characterization effort is twofold; one aspect centers on correlating the film properties (adhesion, grain size and orientation, porosity, topography, composition and hardness) with the deposition parameters (ion type, ion-beam intensity, ion energy, metal-vapor type, deposition rate, film thickness, deposition temperature, substrate type and surface roughness). The other aspect focuses on characterizing the wear scars of worn surfaces to determine which wear mechanism(s) occurs as a function of wear conditions and surface treatment. Techniques such as SEM and TEM coupled with EDS and WDS analysis will provide information on the film composition and microstructure. An in-situ (SEM) microindenter together with conventional microhardness indenters will provide information on the hardness of modified surfaces. The surface topography and wear-scar profile will be quantified using a high-resolution surface profilometer. During FY 1990, the use of these techniques will continue to characterize the behavior of IBAD Ag coatings on $Al_2O_3$, and other coatings such as Co-Re and Mo-Re oxides and borides, as well as Ti oxides.

Keywords: Ion-Beam-Assisted Deposition, Wear Scars, Modified Surfaces

110. Wear-Machinability Relationships in Intermetallic Alloys

FY 1990
$153,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
ORNL (Contract No. DE-AC05-840R21400) Contact: Peter Blau, (615) 574-1514

Ductile intermetallic alloys such as nickel and ion aluminides have been developed at ORNL for high temperature, corrosive environments. The machinability of these new alloys is now being studied as an important aspect of part fabrication. Issues addressed include high-speed-sliding effects, high-load effects, frictional heating, transfer of materials during contact, and built-up edges on cutting tools. A comparison of sliding and machining of the alloys using several tooling materials including composite ceramics is being conducted using a high-speed, sliding-contact machine built especially for this study. The licensees of the new intermetallic alloys should find the results of this investigation important both in terms of wear applications and component fabrication.

Given the previous background developed on understanding the wear of nickel aluminides, the economically important problem of machining the intermetallic alloys will be attacked. In addition to the nickel aluminides, the new iron aluminides will be included in this work. Issues to be addressed include high-speed-sliding effects, high-load effects, frictional heating, transfer of materials during contact, and built-up edges on cutting tools. A comparison of sliding and machining of the alloys using several tooling materials including composite ceramics will be conducted using a high-speed, sliding-contact machine to be built especially for this study. The second year of this effort will include the important effects of metalworking lubricants. The licenses of the new intermetallic alloys should find the results of this investigation important both in terms of wear applications and component fabrication.

Keywords: Intermetallic Alloys, Friction, Wear

111. Thermochemical Surface-Damage Model for Ceramics — FY 1990 $50,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
Georgia Institute of Technology (ORNL Subcontract 780219X-15) Contact: Ward Winer, (404) 894-3270

This project focuses on investigating the effect of lubricant compositions on the wear of several advanced ceramics, including partially stabilized zirconia, silicon nitride, silicon carbide, sialon, and possibly a superconducting ceramic compound. Wear tests include rolling-element EHD tests and pin-on-disc tests under lubricated conditions and temperatures up to 150 °C. This activity has made contributions to the understanding of frictional heating phenomena related to the onset of surface damage in ceramics. Internationally recognized successes have included the development of real-time hot-spot observations and infra-red mapping systems. Surface-damage-control maps for various combinations of sliding speed and contact stress have been developed for dry contacts and are currently being extended to lubricated contacts. The surface-damage maps will incorporate fracture criteria, and lubricated indentation experiments will develop the necessary baseline data to support this analytical treatment.

Keywords: Ceramics, Wear, Friction, Lubrication

112. Additive Response of Base Oils — FY 1990 $50,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
National Institute for Standards and Technology: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

Base oils are composed of many organic molecular structures that may function independently, synergistically, or antagonistically to affect the performance of the lubricants.

Furthermore, lubricating oil additives respond differently in different base oils, due to the interactions between the additives and the base oil constituents. Basic structural information and the types of interactions with additives will help in future development of advanced lubricants.

The goal of this activity is to obtain structural information on base oils to aid in the development of future advanced lubricants, will be attempted by separating lubricating base oils into their major fractions and subfractions, chemically analyzing these fractions and characterizing the tribological performance of these compound classes in friction, wear and oxidation tests. The additives are then tested with the fractions to identify what causes synergism and what causes antagonism. Finally, model compounds selected on the basis of the research on the fractions will be obtained and used to verify the findings. If the chemical species in the base-oil fractions which are beneficial to lubrication can be identified, separated and fed back to the distillate stream, this will increase lubricant supply, conserve energy (direct), and achieve better lubricants (indirect energy savings). As the chemistries in the base oils are identified and understood, novel chemistries of new additives based on these results will lead to new additive technology.

Keywords: Base Oils, Additives, Lubricants, Friction, Wear

113. Advanced Materials/Lubricant Interactions — FY 1990 $135,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
National Institute for Standards and Technology: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

Advanced materials such as ceramics, superalloys and coatings are being used increasingly in various applications requiring wear resistance under severe environmental conditions. Data obtained at NIST and those reported in the literature indicate that the wear rate and the friction coefficient of many advanced materials are generally too high for achieving material conservation or energy conservation. In order to successfully utilize these materials, lubricants must be developed to control friction and wear.

An objective of this activity is to investigate the fundamental mechanisms involved in the interactions between various synthetic base oils, additives and ceramics to generate information that would allow lubricants to be designed for future engine systems that utilize ceramic components. Specifically, the role of the ceramic surfaces on the tribochemical reactions leading to the formation of lubricating films, the effect of the substrate on the thermo-oxidative chemistry of the lubricant, and the effect of lubricant chemical structure will be determined and the reaction kinetics established. The effect of sintering aids on the formation of ceramic-lubricant interaction products will be investigated. Initial research will emphasize SiC, $Si_3N_4$ and alumina.

Ceramic coatings are being considered as thermal barrier insulating layers on the inside surfaces of the cylinder walls of LHR engines. The critical factor in determining the success of these engines lies in the control of friction and wear at the contact between the ceramic coatings and the piston ring. Ceramic coatings are also being considered for other critical areas such as the valve seats. Yet, there are no reliable test methods available for evaluating the friction, wear and ultimate life of these coatings. An activity is underway to develop a test procedure for evaluating the performance of ceramic coatings for tribological applications. This research will be conducted in close cooperation with Caterpillar and Cummins Engine. The ceramic coatings will be selected based on the present knowledge and experience of these two companies, acquired in the development of the LHR engine. The results of the research will be evaluated to gain an understanding of the behavior of ceramic coatings as well as for developing new performance test procedures.

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

114. Liquid Lubricants for Advanced Heat Engines — FY 1990 $160,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
National Institute for Standards and Technology: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

Successful implementation of advanced engine designs, such as the low-heat-rejection engine (LHRE), is hindered by the lack of stable lubricants and additives for high-temperature applications. Current engine technology is the result of years of materials and lubricants research and development. Extensive experience on metals, alloys, lubricants and additives has evolved from this process. However, extension of this experience to new technological areas has been slow. A major factor is that most conventional lubricant applications involve regimes of 200 °C or lower and the understanding for extension of the knowledge gained to the temperature requirements for future advanced systems is lacking. The temperatures in the LHRE may exceed 400 °C and have a top-ring-reversal temperature as high as 425 °C. The need is for lubricants with the capability to effectively survive the severe thermo-oxidative environment, minimize deposit formation and still control friction and wear. A critical component to success in this area is the development of information and an understanding of high-temperature science involving new chemical additives and lubricants.

In cooperation with industry, the goal is to develop a superstable liquid lubricant for heat engines capable of surviving for a minimum of seven minutes at 245 °C (800 °F). Test methods will be developed to identify key structural and chemical requirements for stable lubricants, evaluate base stocks and additives using these methods and work cooperatively with industry in the development of a lubricant for the LHRE.

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

115. Chemiluminescence of High-Temperature Additives

FY 1990
$80,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
National Institute for Standards and Technology: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

In developing new antioxidants for high-temperature applications, conventional chemistries such as hindered phenols, amines, and sulfur compounds are not adequate. New chemistries, however, are difficult to evaluate and develop. Conventional oxidation testing usually gives only go/no-go feedbacks. Chemiluminescence offers an approach for monitor the effectiveness of additives to react with free radicals of other active species enabling an assessment of their capability to control oxidation reactions at high temperatures. The knowledge-base developed will be applicable to the development of lubricants with adequate high-temperature stability.

Chemiluminescence (CL) is a rapid, versatile and non-intrusive technique that allows continuous monitoring of low or high rates of oxidation. Therefore, both storage and service conditions could be simulated or directly observed. In addition to providing relative information on fuel and lubricant oxidation stability and the effects of catalysts or inhibitors, properly designed CL test methods could yield fundamental information on oxidation kinetics and reaction mechanisms. It is the goal of this activity to explore the use of the chemiluminescence technique to monitor the generation and subsequent control of free radicals of lubricants under oxidative/thermal attack. The NIST system design will be modified to enable different molecular structures to be explored for effective lubricant-life control in the 200 °C to 300 °C temperature range, and to develop data on free-radical mechanisms on a molecular level in complex systems.

Keywords: Chemiluminescence, Oils, Friction, Wear, Engines

## Technology Transfer and Management Coordination

116. Management and Coordination (WBS No. 111)

FY 1990
$825,000

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

The objective of this effort is to assess the ceramic technology needs for advanced automotive heat engines, formulate technical plans to meet these needs, and prioritize and implement a long-range research and development program.

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

117. International Exchange Agreement (IEA) Annex II Management and Support (WBS No. 4115)

FY 1990
$708,000

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

The purpose of this effort is to assist and encourage international cooperation in the development of voluntary standard methods for determining mechanical, physical, and structural properties of advanced ceramic materials. There are four tasks in the Annex II agreement, "Cooperative Program on Ceramics for Advanced Heat Engines and Other Conservation Applications," 1) technical information exchange, 2) ceramic powder characterization, 3) ceramic chemistry, and 4) ceramic material property measurements. Research for subtasks 2, 3, and 4 has been completed. Participants in Annex II include the United States, the Federal Republic of Germany, Sweden and, most recently, Japan.

Two new subtasks, Subtask 5 - Tensile and Flexural Properties of Ceramics and Subtask 6 - Advanced Ceramic Powder Characterization, have been added.

Keywords: IEA, Powder Characterization, Mechanical Properties

118. Standard Reference Materials (WBS No. 4116)

FY 1990
$309,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: S. Malghan, (301) 975-2000

This project is directed toward a critical assessment and modeling of ceramic powder characterization methodology and toward the establishment of an international basis for standard materials and methods for the evaluation of powders prior to processing. There are three areas of emphasis: 1) to divide, certify, and distribute five ceramic powders for an international round-robin on powder characterization; 2) to provide reliable data on physical (dimensional), chemical, and phase characteristics of two silicon nitride powders (a reference powder and a test powder); and 3) to conduct a statistical assessment and modeling of round-robin data. The round-robin is to be conducted through the auspices of the International Energy Agency.

Keywords: IEA, Reference Material, Powder Characterization

Device or Component Fabrication, Behavior or Testing

119. Ceramic Component Design Technology

FY 1990
$100,000

DOE Contact: Saunders B. Kramer, (202) 586-8000
NASA Contact: John Gyekenyesi, (216) 433-3210

The advanced finite element and probability codes required to design, analyze and optimize ceramic components are being developed. Enhancement of the CARES code to include the design methods for whisker toughened ceramics was begun in 1989.

Keywords: Probabilistic Computer Codes, Ceramic Component Design

120. Life Prediction Methodology (WBS No. 3222)

FY 1990
$763,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: C. R. Brinkman, (615) 574-5106
Allison Gas Turbine Division Contact: D. L. Vaccari, (313) 230-4313

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

Keywords: Life Prediction, Nondestructive Evaluation, Structural Ceramics

121. Life Prediction Methodology (WBS No. 3223)

FY 1990
$546,000

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

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

Keywords: Life Prediction, Nondestructive Evaluation, Structural Ceramics

122. Component Testing (WBS No. 3316) — FY 1990 $39,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Garrett Ceramic Components Division Contact: M. V. Mitchell, (213) 618-6579

Garrett is planning to fabricate fuel pump push rod ends, valve spring seats, and tappet rollers from GS-44, a gas-pressure sintered silicon nitride. The components will be tested in actual race car engines, test results will be analyzed, and a report prepared.

Keywords: Fabrication, Component Test, Silicon Nitride

123. Component Testing (WBS No. 3317) — FY 1990 $27,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Carborundum Contact: Roger S. Storm, (716) 278-2544

Carborundum is planning to fabricate fuel pump push rod ends from their sialon composition. Several components will then be tested in a high-speed spin fixture and components shall be inspected to obtain wear rate data. Components shall then be assembled in a race car engine and tested using a dynamometer. Again, post-test inspection shall be conducted to determine wear rate data. Following successful completion of this stage of testing, one or more of the components shall be assembled in an engine and installed in several race car applications. Wear data will be collected after completion of racing and engine overhaul pending availability of the fuel pump push rods from the race cars. Data shall be analyzed and evaluated and a report prepared.

Keywords: Fabrication, Component Test, SiAlON

124. Component Testing (WBS No. 3318) FY 1990 $53,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Detroit Diesel Allison Contact: K. E. Weber, (313) 592-7224

The objective of this project is to inspect and test 100 domestically produced silicon nitride cam-roller followers built to the requirements of Detroit Diesel's Series 60 4-cycle, 275-400 hp diesel engine. The inspections and functional laboratory tests shall be equal to those previously conducted on foreign-produced cam-roller followers and the results compared in a report.

Keywords: Fabrication, Component Test, Silicon Nitride

125. Component Testing (WBS No. 3319) FY 1990 $33,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
Norton/TRW Contact: T. G. Kalamasz, (603) 894-6775

Two engine sets of intake and exhaust valves shall be fabricated using a pressureless sintered silicon nitride material. A high speed motored test rig shall be utilized to characterize valve train dynamics of the standard NASCAR valve train set-up and a set-up with ceramic valves. A firing engine dyno test will be performed to quantify changes in engine performance as a result of using ceramic valves and reduced load springs. The standard engine with metal valves shall be used as a baseline for the performance testing. Quantification of the wear benefits of ceramics and a demonstration of their reliability using extended tests will be performed. Data from dynamics performance, wear, and durability testing shall be analyzed and results summarized in a SAE paper.

Keywords: Fabrication, Component Test, Silicon Nitride

126. Ceramic Component NDE Technology FY 1989 $100,000

DOE Contact: Saunders B. Kramer, (202) 586-8000
NASA Contact: Alex Vary, (216) 433-6019

The objective is to identify and develop NDE techniques for ceramic heat engine components. The NDE methods under study are X-ray, radiography, ultrasonics, scanning laser acoustic microscopy and thermo-acoustic microscopy.

Keywords: Ceramics, NDE, X-ray, Ultrasonics

127. Ceramic Mechanical Property Test Method Development (WBS No. 4121)

FY 1990
$200,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
National Institute of Standards and Technology (NIST) Contact: G. Quinn, (301) 975-5765

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

Keywords: Test Procedures

128. Advanced Coating Technology (WBS No. 1311)

FY 1990
$175,000

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

The objective of this project is to develop an adherent coating that will prevent sodium corrosion and provide simultaneous oxidation protection of silicon nitride, silicon carbide, or other ceramics used as components in gas turbine engines.

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

129. Advanced Coating Technology AGT (WBS No. 1312)

FY 1990
$415,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. Ray Johnson, (615) 576-6832
GTE Contact: H. Rebenne, (617) 466-2528

The objective of this project is to develop oxidation-resistant, high toughness, adherent coatings for silicon-based ceramic substrates, namely reaction bonded $Si_3N_4$ sintered SiC, and HIPed $Si_3N_4$ for use in an advanced gas turbine engine. Chemical vapor deposition (CVD) is being used to develop appropriate coating configurations to accommodate as many of the mechanical, thermal, and chemical requirements demanded of the application as possible.

A Phase II effort comprised of three major tasks: 1) optimization and modification of the coating configuration; 2) performance assessment; and 3) modeling was initiated in FY 1989.

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

130. Wear Resistant Coatings (WBS No. 1331) FY 1990 $112,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Caterpillar Contact: C. D. Weiss, 309-578-8672

The goal of this project is to develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically, piston rings and cylinder liners. Three coating processes, plasma spraying, vapor deposition (CVD-PVD), and enameling, are being investigated to develop adherent, wear-resistant ceramic coatings. The coating systems will be screened for wear and friction at 350 °C under lubricated conditions. Coatings which show promise will be optimized by adjustments to chemistry and hard particle content to meet the wear and friction goals. Optimized coatings will then be fully characterized for oxidation, adherence, uniformity, thermal shock, wear, and friction. Selected coatings will be applied to simulated engine component specimens and thermal conductivity measurements will be obtained.

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

131. Wear Resistant Coatings (WBS No. 1332) FY 1990 $ 0

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: D. P. Stinton, (615) 574-4556
Cummins Contact: Malcolm Naylor, (812) 377-7713

The goal of this project is to develop wear-resistant coatings for application to metallic components of low-heat-loss diesel engines, specifically, piston rings and cylinder liners. Visual inspection and oxidation; friction and wear tests; thermal shock uniformity, hardness, and adherence; and electron microscopy and surface analysis will be evaluated to determine the chemical and microstructural characteristics that control the coatings' wear, adherence, and reliability. Based on a review of the data, the most promising coating systems will be selected for further evaluation.

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

132. Active Metal Brazing PSZ-Iron (WBS No. 1411) FY 1990 $243,000

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

The objective of this task is to develop strong reliable joints containing ceramic components for applications in advanced heat engines. A novel method for brazing zirconia to cast iron has already been established. Presently, this work is focused on the joining of silicon nitride by brazing. Current efforts include high temperature brazing of titanium vapor-coated silicon nitride, correlating braze joint microstructures with strength data to identify factors controlling joint strength, and developing a method of calibrating the indentation fracture technique to determine the accuracy of residual stresses measurements in ceramic-to-metal joints.

Keywords: Metals, Structural Ceramics, Joining/Welding, Brazing, Cast Iron, Zirconia, Alumina, Silicon Nitride

133. Metal-Ceramic Joints AGT (WBS No. 1412) FY 1990 $296,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
GTE Contact: S. Kang, (617) 890-8460

The goal of this work is to demonstrate analytical tools for use in designing ceramic-to-metal joints including the strain response of joints as a function of the mechanical and physical properties of the ceramic and metal, the materials used in producing the joint, the geometry of the joint, externally imposed stresses both mechanical and thermal in nature, temperature, and the effects on joints exposed for long times at high temperature in an oxidizing (heat engine) atmosphere. The technical work involves both analytical and experimental tasks. The goal of the analytical work is a predictive model that can be used in engineering design of ceramic joints. The experimental work will involve the fabrication and testing of first small scale and later scale-up sized joints.

Keywords: Engines, Joining/Welding, Metals, Structural Ceramics, AGT, Metal-Ceramic, Physical/Mechanical Properties

134. Metal-Ceramic Joints AGT (WBS No. 1413) FY 1990 $43,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
Battelle Contact: A. T. Hopper, (614) 424-4567

The objective of this project was 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 involved both analytical and experimental tasks. The goal of the analytical work was a predictive model that can be used in engineering design of ceramic joints. A PC-based computer program for ceramic-ceramic and ceramic-metal joint design and assessment has been completed. The user friendly computer code allows quick analysis of joints between various materials. Experimental verification tests confirmed excellent agreement between predictions and experimental data.

Keywords: Engines, Joining/Welding, Metals, Structural Ceramics, Modeling, Oxides

135. Ceramic-Ceramic Joints AGT (WBS No. 1421) FY 1990 $350,000

DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: M. L. Santella, (615) 574-4805
Norton Contact: G. A. Rossi, (508) 393-5829

The purpose of this program is to develop techniques for producing reliable ceramic-ceramic joints and analytical modeling to predict the performance of the joints under a variety of environmental and mechanical loading conditions including high temperature, oxidizing atmospheres. The ceramic materials under consideration are silicon nitride and silicon carbide. The joining approach for silicon nitride is based on the ASEA hot isostatic pressing process, while the plan is to co-sinter silicon carbide green forms together. These joining methods were selected to produce joints which exhibit the minimum possible deviation in properties from those of the parent ceramic materials. Analytical models will be experimentally verified by measurements on experimental size and scale-up joints as part of this work.

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

136. Thick Thermal Barrier Coatings FY 1990
$25,000

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

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

Keywords: Coatings, Oxide Ceramics, Diesel Engines

137. Thick Thermal Barrier Coatings FY 1990
$135,000

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

Zirconia thermal barrier coating (TBC) systems are being developed and applied to diesel engine parts for evaluation in a single cylinder engine rig. Initial evaluation of engine tests indicated deterioration by combustion possibly attributed to TBC coating porosity and surface roughness. These problems are being further investigated.

Keywords: Coatings, Oxide Ceramics, Diesel Engines

138. Advanced Diesel Engine Component Development Project FY 1990
$75,000

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

The objective of the project is to develop advanced technology diesel engine components and integrate these into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative, and tribological component applications.

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

139. Advanced Piston and Cylinder Component Development FY 1990 $500,000

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

The objective of the project is to develop advanced technology diesel engine components and integrate these into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative, and tribological component applications.

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

140. Advanced Piston and Cylinder Component Development FY 1990 $500,000

DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: J. J. Notardonato, (216) 433-3908
Cummins Engine Contact: D. H. Reichenbach, (812) 377-7041

The objective of the project is to develop advanced technology diesel engine components and integrate these into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative and tribological component applications.

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

141. High Temperature Solid Lubricant Coatings FY 1990 $50,000

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

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

Keywords: Wear, Coatings, Diesel Engines, Tribology

142. Advanced Turbine Technology Applications Project (ATTAP, AGT-5) FY 1990
$5,100,000

DOE Contact: Saunders B. Kramer, (202) 586-8000
NASA Contact: Paul Kerwin, (216) 433-3409;
General Motors, Allison Gas Turbine Division, Contact: Phil Haley, (317) 230-2272

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

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

143. Advanced Turbine Technology Applications Project (ATTAP, AGT-101) FY 1990
$5,100,000

DOE Contact: Saunders B. Kramer, (202) 586-8000
NASA Contact: Thomas N. Strom, (216) 433-3408
Garrett Turbine Engine Contact: Jim Kidwell, (602) 220-3463

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

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

144. IBAD Tribological Characterization FY 1990
$260,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
ANL (Contract No. W-31-109-ENG-38) Contact: Fred Nichols, (312) 972-8292

The tribological evaluation effort focuses on measuring the friction and wear properties of surface-modified substrates as a function of temperature, load, sliding velocity and sliding distance. Several pieces of equipment will be used for these tests depending on the desired temperature, load, velocity and environment. During FY 1990, a new test apparatus capable of testing ring-on cylinder configurations at elevated temperatures will be designed and constructed. This system is necessary to test components with loads and geometries more prototypical of ring/cylinder geometry than the pin-on-disc/flat configurations currently in use.

Keywords: Surface Modification, Ring/Cylinder Wear, Friction, Wear

145. Energy-Efficient Gear-Lubrication Model — FY 1990 — $50,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
Northwestern University (NIST Subcontract No. 60NANBD0547) Contact: Herbert Cheng, (312) 491-7062

The main objectives in this activity conducted at Northwestern University include modeling of friction and wear in the partial elastohydrodynamic lubrication regime, calculations of power loss and wear loss in spur gears and experimental validation of the friction and wear models. This work is expected to aid the development of new lubricants for more energy-efficient power transmission. Initial project work has led to the development and preliminary experimental validation of a model for predicting gear friction and resultant power loss. In FY 1990, validation of this model was completed and a model for predicting wear in spur gears successfully developed.

Keywords: Gears, Oils, Friction, Wear, Engines

146. Lubrication Model — FY 1990 — $75,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
National Institute for Standards and Technology: Gaithersburg (Interagency Agreement OR-21350) Contact: Stephen Hsu, (301) 921-2113

Effective lubrication of actual components involves fluid-film support, chemical-film formation, oxide-layer protection and material properties. Prediction of lubricated wear therefore is very complex and involves fluid mechanics, materials science, chemistry and the physics of the contact. Current models are segregated along disciplinary lines, and hence are of limited use. This project is structured to bring fluid mechanics, surface chemistry, materials science and lubricant-oxidation/degradation phenomena together to develop an *a priori* model. The objective is to develop a validated model for predicting the lubrication limits and wear life of simple materials under idealized contacting conditions by assembling various current expertise, and by developing a conceptual model to link all critical factors involving chemical and material-property control in the contact zone.

Keywords: Lubrication, Wear, Wear Life

147. Wear Mechanism Modeling

FY 1990
$72,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
Cambridge University Contact: M. F. Ashby, 0-223-33-2-2622

In the study of tribology, investigators often employ different wear/friction test geometries and conduct tests at different pressures and speeds, with little or no effort to correlate the results of different tests. Often variable wear mechanisms occur under different conditions, complicating the prediction of tribological performance and properties. A recent technique published by Lim and Ashby uses normalized coordinates to correlate, in a surprisingly consistent manner, an extremely large and varied data base on steel-on-steel studies. This project, initiated in FY 1989, extends the Lim and Ashby treatment to include arbitrary combinations of wear/friction pairs with differing material properties. In FY 1989, a technique was developed for calculating both bulk and flash temperatures due to frictional heating and fitting. During FY 1990 these calculations were further refined and applied to the analysis of various ceramic/metal wear couples.

Keywords: Metals, Ceramics, Friction, Wear, Engines

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

FY 1990
$ 0

DOE Contact: J. J. Eberhardt, (202) 586-1694
MIT Contact: John Heywood, (617) 253-2243

A novel laser fluorescence technique was recently developed at MIT, which measures oil film thickness between the cylinder liner and the piston rings in a reciprocating diesel engine. The laser diagnostic engine study provides *in situ* real time lubricant measurements, an improvement over many advanced fundamental research techniques which are based on bench experiments. It is also known that some tribochemical reactions occur under instantaneous conditions, which can be best addressed with *in situ* engine experiments. The goal of this activity is to establish a model of lubricant flow and residence time at top-ring reversal and in the top-ring zone of a typical top-tight-land-piston configuration similar to those used in prototype low heat rejection engines. The basic differences in oil-film characteristics of a production diesel engine with different lubricants and piston-ring designs will be determined and a simple model of the flow and residence time at top-ring reversal and in the top-ring area developed. The availability of a model will contribute to the ability to establish lubricant criteria for high-temperature liquid lubricants. It will, when coupled with other laboratory-method evaluations and bench scale studies of lubricants, enable more accurate predictions of the performance of a lubricant in current and future engines.

Keywords: Metals, Oils, Friction, Wear, Engines, Laser Fluorescence, Films

149. Effect of Cycle-to-Cycle Variations on Instantaneous Friction Torque FY 1990
$0

DOE Contact: J. J. Eberhardt, (202) 586-1694
Wayne State University (ANL Subcontract No. 73072401) Contact: Naeim Henein, (313) 577-3887

A project involving a new technique to evaluate instantaneous friction torque (IFT) in an operating, reciprocating internal-combustion engine, is in its second year at Wayne State University. This project is jointly funded by NSF and the OTT/OTM Tribology Program with the bulk of the work supported by NSF in a 3-year grant to Wayne State. The OTT Tribology program is only supporting research on "The Effect of Cycle-to-Cycle Variations on the Accuracy of the Instantaneous Friction Torque Determined by the (P-$\omega$) Method." The method itself is being developed in the NSF-funded project.

The OTT-supported work includes and has the prime objective of conducting in-engine testing of surface-modified components developed in an OTT Tribology project at ANL. Initial activities in this project involved a careful and quantitative evaluation of commercially available instrumentation for the measurement of angular velocity, pressure and torque. Based on this evaluation, optimal instrumentation was selected, acquired and installed in the experimental engine.

Keywords: Friction, Torque, Engines, Combustion, Modeling

150. Surface Roughness Wear Model for Ceramics FY 1990
$40,000

DOE Contact: J. J. Eberhardt, (202) 586-1694
SKF-MRC, Inc. (Contract No. DE-AC02-87CE90001) Contact: John McCool, (215) 889-1300

This project conducted at SKF-MRC, Inc., with support from ORNL and ANL, has resulted in the development of a personal computer-based software package (RUFFIAN) which predicts wear and load-bearing area, and aids in surface finish selection for ceramic bearings. The program was validated in FY 1989 based on testing support from ORNL and ANL. The computer software development work has also led to the ability to estimate frictional flash temperatures. Experimental validation of the modeling concepts concluded with a final analysis and final report in FY 1990.

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

151. Glassy-Carbon Materials for Severe Wear Environments FY 1990
$ 0

DOE Contact: J. J. Eberhardt, (202) 586-1694
Burton Technologies, Inc. (Contract No. DE-AC02-88CE90027) Contact: R. A. Burton, (919) 839-8287

Initial evaluation of a low-wear, vitreous-carbon material demonstrated wear rates that are lower than many ceramics and low, steady friction coefficients. The glassy carbon had none of the environmental sensitivity normally experienced by carbon-based materials like graphite when used in sliding dry air. Test specimens will be fabricated by Burton Technologies and provided to ORNL for testing in a high-speed sliding machine constructed to impose severe sliding conditions such as might be encountered in mechanical face seals and engine components. Burton Technologies will also conduct mechanical face-seal simulator tests in their laboratory. Correlations between these two testing geometries will be drawn. The behavior of the glassy carbon will be compared to that of metals and ceramics subjected to the same severe conditions. This work should open up new applications for the vitreous-carbon materials. This work will be completed in FY 1990.

Keywords: Glassy-Carbon Materials, Tribology, Friction, Wear

## OFFICE OF UTILITY TECHNOLOGIES

The Office of Utility Technologies formulates, articulates, executes, and evaluates a national program of technology planning, research and development, and test and evaluation for utility technologies.

In addition, the Office is responsible for the development, execution, and evaluation of program specific technology transfer programs and activities to effect timely transfer of technology from Federal laboratories to energy production concerns, and facilitate informed decision-making within the energy utilization community.

Materials research within the Office of Utility Technologies is carried out by the Office of Solar Energy Conversion, the Office of Renewable Energy Conversion and the Office of Energy Management.

### Office of Solar Energy Conversion

The mission of the Office of Solar Energy Conversion is to provide overall direction, interpret policy objectives, and establish management procedures for a balanced program of technology planning, research, development, test, analysis, evaluation, and communication that will foster the establishment of solar energy supply options for use by utilities and allied industries and institutions.

The Office represents, as the national programmatic expert, the photovoltaic and solar thermal and biomass power—technologies in the formulation and execution of national energy policies and programs. The Office is responsible for the establishment of program balance and priorities among subordinate Divisions.

### Solar Thermal and Biomass Power Division

The mission of the Solar Thermal and Biomass Power Division is to plan and manage a balanced program for technology research, development, testing and evaluation which will foster the establishment of solar thermal energy and biomass power technology supply options.

The Division serves as the national federal technical expert for the purpose of formulating and executing national energy policies and programs relating to solar thermal and biomass power technologies.

Materials Preparation, Synthesis, Deposition, Growth or Forming

152. Silver/Polymer Reflector Research

FY 1990
$850,000

DOE Contact: Martin Scheve, (202) 586-8110
SERI Contact: Gary Jorgenson, (303) 231-1226

Research and development of silver/polymer reflector films for solar thermal systems was conducted. For solar thermal applications, the silvered films must be resistant to ultraviolet degradation, cleanable, and have specular reflectances of 90 percent or more, with a 4 mrad cone angle. Useful film lives of 5 years or longer are needed.

Solar concentrators account for about 50 percent of the installed cost of a solar thermal electricity or process heat system. Silvered polymer films offer lower cost, reduced weight, and greater design flexibility than silver on glass.

Research continued on characterization, testing, and evaluation of a variety of ultraviolet stabilized silver/polymer films. New efforts focused on environmental concerns such as delamination and ease of field replacement on concentrators, as well as on evaluation of different suppliers to reduce polymer cost.

Keywords: Polymers, Coatings and Films, Surface Characterization and Treatment, Corrosion, Radiation Effects, Reflectors, UV Degradation

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

153. Amorphous Silicon for Solar Cells

FY 1990
$8,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: Richard Crandall, (303) 231-1913

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

154. Polycrystalline Thin Film Materials for Solar Cells

FY 1990
$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

155. Deposition of III-V Semiconductors for High-Efficiency Solar Cells — FY 1990 $2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
SNLA Contact: David Hasti, (505) 844-8161

This project performs applied research upon deposition of III-V semiconductors for high efficiency solar cells, both thin film for flat plate applications and multilayer cells for concentrator applications. Research centers upon depositing layers precisely controlled in terms of composition, thickness and uniformity and studying the interfaces between the layers. The materials are deposited by chemical vapor deposition, liquid phase epitaxial growth and molecular beam epitaxial growth. The long term goal of this area is to develop 35 percent efficient concentrator cells and 24 percent 100 $cm^2$ one-sun cells for flat plate applications. Achieving these goals would enable systems using these technologies to be cost-effective electrical generators.

Keywords: Semiconductors, Chemical Vapor Deposition, Solar Cells (Liquid Phase Epitaxial Growth, Molecular Beam Epitaxial Growth)

Materials Properties, Behavior, Characterization or Testing

156. Materials and Device Characterization — FY 1990 $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

157. High-Efficiency Crystal Silicon Solar Cells

FY 1990
$2,000,000

DOE Contact: Morton B. Prince, (202) 586-1725
SERI Contact: John Benner, (303) 231-1396
SNLA Contact: David Hasti, (505) 844-8161

This project performs applied research upon crystal silicon devices to improve solar-to-electric conversion efficiency. The project employs new coatings and/or dopants and other treatments to reduce electron-hole recombination at cell surfaces or in the bulk material. This project also performs applied research upon the growth of silicon ribbons from a melt. Research centers upon understanding, from a physical perspective, exactly what happens during the growth of silicon ribbon. Questions to be answered include: what stresses do the sharp temperature gradients, inherent in high speed crystal growth impose upon the ribbon; which stress relief modes improve solar cell performance and how can they be enhanced; how can buckling be prevented; and what is an acceptable level of residual strain.

Keywords: Semiconductors, Solar Cells

Office of Renewable Energy Conversion

The mission of the Office of Renewable Energy Conversion is to provide overall direction, interpret policy objectives, and establish management procedures for a balanced program of technology planning, research, development, test, analysis, evaluation, and communication that will foster the establishment of renewable or alternate energy supply options for use by utilities and allied industries and institutions.

The Office represents, as the national programmatic expert, the wind, hydropower, oceans and geothermal technologies in the formulation and execution of national energy policies and programs. The Office is responsible for the establishment of program balance and priorities among subordinate Divisions.

Geothermal Division

The mission of the Geothermal Division is to plan and manage a balanced program for technology research, development, testing and evaluation which will foster the establishment of geothermal technology supply options.

The Division serves as the national federal technical expert for the purpose of formulating and executing national energy polices and programs relating to geothermal technology.

Materials Preparation, Synthesis, Deposition, Growth or Forming

158. Materials for Non-Metallic Heat Exchangers

FY 1990
$85,000

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

This project is investigating thermally conductive polymer-based composites for use as corrosion resistant materials of construction for shell and tube heat exchangers in binary geothermal processes or for liners on carbon steel substrates. Corrosion of the brine side of tubing in shell and tube heat exchangers has been a major problem in the operation of binary geothermal processes. Compared to the cost of high alloy steels, a considerable economic benefit could result from the utilization of a proven corrosion resistant polymer concrete material if sufficient heat transfer and anti-fouling properties can be derived. The work consists of determinations of the effects of compositional and processing variables on the thermal and fouling properties of the composite, and measurements of the physical and mechanical properties after exposure to hot brine and isobutane/isopentane mixtures. If the goals of the program are attained, the cost of geothermal power from binary processes will be reduced considerably.

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

159. Biochemical Concentration and Removal of Toxic Components from Geothermal Wastes

FY 1990
$200,000

DOE Contact: G. J. Hooper, (202) 586-1146
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 microorganisms 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

160. Advanced High Temperature Geothermal Well Cements — FY 1990 $155,000

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

Lightweight (<1.2 g/cc) chemically and thermal resistant well cements are needed to reduce the potential for lost circulation problems during well completion operations. Materials designed for temperatures >500 °C will be needed as higher temperature resources are developed. Cements resistant to brines containing high concentrations of $CO_2$ at temperatures >150 °C are also needed. Emphasis is being placed on high temperature rheology, phase chemistry, and the mechanical, physical, and chemical resistance properties of the cured materials.

Keywords: Cements, Material Degradation, Strength, Transformation, Bulk Characterization, Drilling, Carbonation

161. Corrosion in Binary Geothermal Systems — FY 1990 $4,700

DOE Contact: R. LaSala, (202) 586-4198
BNL Contact: D. van Rooyen, (516) 282-4050

This program yields corrosion data from plant tests for metals presently used in binary plants and other more potentially resistive metals and nonmetals. In operating binary processes, brine leakage into the organic working fluid side of the plants has resulted in unanticipated corrosion problems. Data are not available on the effects of salt, oxygen, and water impurities in isobutane and/or isopentane on the corrosion rates of metals. The work involves the exposure of test coupons in an operating plant. When completed, the program will yield quantitative information regarding the extent of corrosion that will occur upon contamination of the binary side of a plant, thereby allowing designers materials options.

Keywords: Alloys, Metals, Corrosion

162. Advanced High Temperature Chemical Systems for Lost Circulation Control

FY 1990
$95,000

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

The cost of correcting lost circulation problems occurring during well drilling and completion operations constitutes 20 to 30 percent of the cost of a geothermal well. The objective of the program is to develop an advanced high temperature chemical system which when added to bentonite-based drilling fluids will produce a slurry which is pumpable at high temperature and which upon curing will yield an expandable high strength brine-resistant cementitious material. Emphasis is being placed upon high temperature rheology, phase chemistry, and the mechanical, physical and chemical resistance properties of the cured material.

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

163. Corrosion Mitigation in Highly Acidic Steam Condensates

FY 1990
$60,000

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

Increased HC1 gas concentrations in the steam produced from geothermal wells at The Geysers in Northern California have resulted in severe corrosion problems in casings in the upper regions of wells where condensation may occur, and in the well-head and transmission piping. The objective of the program is to optimize and field test polymer matrix composites for utilization as corrosion resistive liners on carbon steel components exposed to low pH steam condensates at temperatures up to ~200°C. Emphasis is being placed on composite composition, installation procedures and techniques for joining lined pipe sections.

Keywords: Polymer Matrix Composites, Acid, Durability, Fabrication Techniques, Field Tests

Office of Energy Management

The mission of the Office of Energy Management is to provide federal leadership for the research and development of new technologies and processes that promote efficiency, reliability, and flexibility in the nation's utility energy delivery systems. The Office manages programs in utility systems and advanced utility concepts and is responsible for leading R&D centers consistent with DOE and CE policies, establishing 5-year program goals, consolidating organizational units to focus resources, and pursuing leveraging opportunities with industry, utilities, and other government agencies by providing technology transfer assistance, encouraging Cooperative Research and Development Agreement (CRADA) establishment, and implementing cost-shared research programs.

Utility Systems Division

The Utility Systems Division supports research and development directed toward solving mid- to long-term problems in electric energy transmission and distribution and promotes the development and integration of new materials, advanced controls, and new design concepts into the utility network. The program supports research activities in the following areas: Integrated Resources Planning, Electric Field Effects, Transmission and Distribution Technologies, and District Heating and Cooling.

Materials Properties, Behavior, Characterization or Testing

164. Gaseous Dielectric Decomposition, Detection, and Mitigation of $S_2F_{10}$ — FY 1990: $ 0

DOE Contact: R. Eaton, (202) 586-1506
Oak Ridge National Laboratory Contact: D. R. James, (615) 574-0266

The objective of the research is to participate in a Cooperative Research and Development Program CRADA to develop detection techniques to permit sensitive detection of $S_2F_{10}$ by investigating the formation and destruction mechanisms, and determining the stability, toxicity, and thermal/chemical properties. The CRADA members are EPRI, ESEERCO, CEA, Ontario Hydro, NIST, and ORNL. The research has determined that $S_2F_{10}$ is produced in corona and spark discharges in $SF_6$, a gas used extensively for electrical insulation and arc extinction. Research goals are to improve detection techniques of $S_2F_{10}$ down to the ceiling value limit, to investigate the formation and decomposition rates of $S_2F_{10}$ in $SF_6$ discharges for different levels of gas impurities and moisture that simulate practical operating environments, and to determine the toxicity of $S_2F_{10}$ after formation in $SF_6$ environments.

Keywords: Sulfur Gas Detection, Chemical Properties, Spark Discharges

165. Pre-Breakdown Events in Liquid Dielectrics — FY 1990: $125,000

DOE Contact: R. Eaton, (202) 586-1506
University of Tennessee Contact: M. O. Pace, (615) 974-5419

The objective of the research is to gain a better understanding of pre-breakdown events critical in breakdown and aging of a dielectric liquid under high voltage stress in order to improve the dielectric strength of liquids, increase aging resistance, and develop appropriate diagnostic and monitoring methods for liquid insulated power equipment. Pre-breakdown current pulses in dielectric liquids which were thought to be random were found to be well-ordered. The pulses originate during the expansion of a low density region at the cathode. The present investigation is concentration on the initiation of this low density region, the nature of its interior, and further identifying the relation to the accompanying current and light pulses. Additional experiments will be made to obtain the spectral composition of the discharge light emission.

Keywords: Liquid Dielectrics, Dielectric Strength, Pre-breakdown Events in Liquid Insulated Power Equipment

Advanced Utility Concepts Division

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

Materials Preparation, Synthesis, Deposition, Growth or Forming

166. Corrosion-Resistant Coatings for High-Temperature, High-Sulfur Activity Applications

FY 1990
$137,000

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

This research project explores electrodeposition and chemical vapor deposition techniques used to prepare corrosion-resistant coatings for high-temperature batteries. The deposition of molybdenum and $Mo_2$-C by electrochemical deposition in molten salt was optimized in order to obtain reproducible thicknesses and smooth surface morphology. The corrosion resistance of Mo, $Mo_2$-C and TiN were determined in Na-polysulfide melt. All three coatings showed behavior comparable to that of solid Mo in this melt.

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

## Materials Structure and Composition

### 167. Molten Salt Cell Research

FY 1990
$275,000

DOE Contact: A. Landgrebe, (202) 586-1483
Argonne National Laboratory Contact: C. Christianson, (312) 972-7563

Experiments are underway to improve the Li-alloy/metal disulfide cell (i.e., to develop separator/electrolyte systems that are stable at high Li activities). High-temperature immobilized electrolyte (HTIE) materials are being investigated for this purpose. These materials consist of an insulator-type ceramic material (e.g., MgO) that is infiltrated by a liquid salt which is held in the pores by capillary forces. The dc conductivity was measured on HTIE separator materials in a specially designed cell and was found to be significantly lower than the conductivity of pure molten salt.

Keywords: Batteries, Solid Electrolytes

### 168. New Battery Materials

FY 1990
$150,000

DOE Contact: A. Landgrebe, (202) 586-1483
Stanford University Contact: R. Huggins, (415) 723-4110

An effort is underway to characterize high-sodium-activity alloys and low-melting-point molten salts for sodium metal chloride cells. This research seeks to improve the removal of the high-impedance solid electrolyte. A number of alloy compositions were screened for their ability to act as fast, reversible sodium-conducting electrodes. The use of a family of alkali halide ammoniate salts for sodium metal chloride cells was also investigated.

Keywords: Batteries, Alloys

### 169. Spectroscopic Studies of Passive Films on Alkali and Alkaline Earth Metals in Nonaqueous Solvents

FY 1990
$52,000

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

Research efforts have focused on preparing and characterizing submonolayer deposits of alkali and alkaline earth metals on metal surfaces and developing the understanding of passive surface layers in rechargeable alkali batteries. The activation of carbon dioxide induced by the presence of alkali metal atoms adsorbed on an otherwise inert substrate was examined with an array of surface analytical methods. The analytical techniques in this study included work function measurements, low energy electron diffraction, Auger electron, X-ray photoelectron XPS, high resolution electron energy loss, and thermal desorption spectroscopies.

Keywords: Surface, Structure, Films, Batteries

170. Raman Spectroscopy of Electrode Surface in Ambient-Temperature Lithium Secondary Battery — FY 1990 $ 0

DOE Contact: A. Landgrebe, (202) 586-1483
Jackson State University Contact: H. Tachikawa, (601) 968-2171

*In situ* Raman spectroscopy was applied to study lithium electrodes in propylene carbonate, 2-methyl tetrahydrofuran and acetonitrile. *In situ* Raman spectroscopic investigations of zinc electrode surfaces were also carried out in 7.0 M potassium hydroxide solutions with and without zinc oxide.

Keywords: Surface, Structure, Batteries

Materials Properties, Behavior, Characterization or Testing

171. High-Temperature Superconducting Materials Pilot Centers — FY 1990 $6,000,000

DOE Contact: R. Eaton, (202) 586-1506
Oak Ridge National Laboratory Contact: A. C. Schaffhauser, (615) 574-4826
Argonne National Laboratory Contact: E. Kaufmann, (312) 972-3606
Los Alamos National Laboratory Contact: R. Quinn, (505) 665-3030

The Pilot Centers were established at three national laboratories (Oak Ridge, Argonne, and Los Alamos) to keep the United States at the forefront of HTS technology research. The laboratories work collaboratively with industry to perform materials research. The laboratories also expedite research efforts by streamlining the process of obtaining patent rights and other intellectual property.

Keywords: Superconductors, Pilot Centers

172. Microfilamentary Superconducting Composite — FY 1990 $288,000

DOE Contact: R. Eaton, (202) 586-1506
Ames Laboratory Contact: D.K. Finnemore, (515) 294-3455

A materials processing technique is being developed to make stabilized microfilamentary superconducting wires suitable for magnets that operate at 35 K. The conductor would carry

10,000 $A/cm^2$ at 5 Tesla with a strain tolerance of 0.5 percent. Tasks include preparation of filament, development of high current transfer at the matrix superconductor boundary, and the study of crystallization as a function of fiber diameter. Babcock and Wilcox has developed an industrial-scale process for producing long, slender fibers of $Bi_2Sr_2Ca_1Cu_2O_8$ by a gas fiberization technique. Researchers have developed fundamental methods for forming superconducting composites by de-beading blown fibers and separating them from the chaff by ultrasonic methods in a volatile fluid, but none of the methods are industrial scale yet.

Keywords: Composites, Fibers, Superconductors, Wires

173. Practical Superconductor Development for Electric Power Applications — FY 1990 $1,246,000

DOE Contact: R. Eaton, (202) 586-1506
Argonne National Laboratory Contact: R. Poeppel, (708) 972-5118

The conductor development program aims to develop methods to fabricate and use structurally reliable HTS conductors in commercially viable electrical energy applications. Emphasis is on low-temperature, non-epitaxial growth of HTS thin films on practical substrates in a manner compatible with continuous fabrication of long wires and tapes. Researchers have made YBCO 124 using low pressure calcination process. Thin films of TBCCO have been post-annealed to achieve $J_c \approx 4x10^4$ $A/cm^2$ at 2 T and 32 K; and thin films of BSCCO with $T_c = 60$ K have been made at low temperatures (700-750 C) in a one-step process. In the area of device development, researchers have made low resistance (below 10 micro-ohm-$cm^2$) electrical contacts and developed insulation for windings using 211 composition YBCO. Electrical coils have been made which generate fields approaching 500 gauss at 77 K.

Keywords: Superconductors, Thin Films, Electrical Contacts, Insulation, Coils

174. Bulk Conductor Development/Device Technology Development — FY 1990 $527,000

DOE Contact: R. Eaton, (202) 586-1506
Brookhaven National Laboratory Contact: D. Welch, (516) 282-3517

The various methods employed for fabricating composite conductors containing high-$T_c$ oxides will be restricted to those which can be scaled up for large scale production for electric power systems applications. Among the candidate methods are: thermal- and plasma-spray coating, rapid solidification and melt processing, and sintered-powder methods. The use of Ag to enhance the sintering process in $YBa_2Cu_3O_7$ was investigated, resulting in improvement in the intergranular weak link behavior but reduction in the intragranular $J_c$. Good progress was made in preparing melt-textured $YBa_2Cu_3O_7$ on a Ni substrate, and flat, rectangular bars textured by this process have $J_c$ of about 1,000 A/cm$^2$ at 8 T and 77 K. A first version of a magnetostatic computer program to compute 2-dimensional quasistatic flux profiles in superconductors has been completed and tested.

Keywords: Composites, Coatings and Films, Structure, Superconductors

175. Thin Films Superconductors for Electric Power Applications — FY 1990 384,000

DOE Contact: R. Eaton, (202) 586-1506
Solar Energy Research Institute Contact: R. McConnell, (303) 231-1019

The purpose is to fabricate thin film based, high-temperature superconductor wires or tapes to carry high currents in electric power system devices. The approach is to identify and develop those thin film fabrication processes suitable for manufacture of long conductors for use in making components for electric power system devices. Researchers are assessing the potential of two relatively novel processes for making superconducting films, electrodeposition and metal organic chemical vapor deposition (MOCVD). Emphasis is on YBCO films, although BSCCO and TCBCO films have also been made. YBCO films as thick as 5 microns are c-axis oriented on epitaxial substrates with $T_c$s of 91 K (2 K width) and initial $J_c$s of 4,000 A/cm$^2$ at 4 K and 360 A/cm$^2$ at 77 K in zero field (as measured at NIST). SERI has completed a MOCVD reactor and fabricated its first MOCVD films. The best MOCVD sample had an onset of 88 K with zero resistance at 55 K.

Keywords: Superconductors, Coatings and Films, Polymers, Structure

176. Bulk and Thin-Film Materials Process Research for High-Temperature Superconductor and Power Device Development — FY 1990 $767,000

DOE Contact: R. Eaton, (202) 586-1506
Sandia National Laboratory Contact: T. Bickel, (505) 844-2392

The purpose of the research is to apply materials research results on bulk and thin-film high-temperature superconductors to the development of improved materials and conductors with properties suitable for use in electric energy systems. Two research tasks are currently underway: Bulk materials and process research on yttrium- and thallium-based HTS powders and thin-film materials research on thallium-based HTS systems. The focus of the research is to increase the critical current density in the presence of magnetic fields to enable the fabrication of practical conductors. The Sandia process for preparing $YBa_2Cu_3O_x$ precursor powders has been demonstrated to produce high-quality, high-temperature superconducting composites on a continuous process scale. Researchers are also studying how processing variables affect mechanical and electrical characteristics of the superconducting powder. The goal is achieving high-density conductors with clean grain boundaries and aligned grain structure. Thin films of materials in the TlCaBaCuO continue to be developed using a film deposition technique of sequential electron beam evaporation followed by *ex situ* sintering and annealing.

Keywords: Superconductors, Crystal Defects and Grain Boundaries, Structure, Consolidation of Powder, Powder Synthesis and Characterization

177. Development and Fabrication of High-Temperature Superconductors

FY 1990
$575,000

DOE Contact: R. Eaton, (202) 586-1506
Los Alamos National Laboratory Contact: D. Peterson, (505) 667-3973

The goal is to fabricate a bulk superconductor with a critical current density of $10^4$ $A/cm^2$ at 35 K and 2 T using efficient and reproducible approaches enabling fabrication of pieces appropriate for uses in power applications. The focus is on using thallium based phases although bismuth and yttrium based materials are also being examined. Researchers developed synthesis routes to obtaining bulk samples of $Tl_2Ba_2Ca_2Cu_3O_{10}$ (Tl-2223), $Tl_2Ba_2CaCu_2O_8$ (Tl-2212) $Bi_2Sr_2CaCu_2O_8$ (Bi-2212), and $YBa_2Cu_3O_7$ (Y-123) were developed. Researchers correlated synthesis parameters with microstructural and electronic properties in order to achieve single phase, high density phases with optimal electronic properties, yielding well characterized samples useful in further processing studies. Hot Isostatic Pressing (HIP) was successfully employed to consolidate a test Y-123 sample to near theoretical density. Rolling experiments were successfully conducted involving production of superconducting Bi-2212 tapes contained within silver foils. Similar rolling studies of Tl-2223 material are underway. Superconducting wires were also fabricated by filling silver tubes with Bi-2212 powder followed by drawing and rolling of tubes. Additional Tl-2223 and Tl-2212 samples were exposed to neutron radiation in an attempt to increase the critical current and introduce flux pinning through local damage.

Keywords: Superconductors, Structure, Films and Coatings, Crystal Defects and Grain Boundaries, Powder Consolidation, Powder Synthesis and Characterization

178. Bulk Conductor Processing and Powder Development

FY 1990
$670,000

DOE Contract: R. Eaton, (202) 586-1506
Oak Ridge National Laboratory Contact: D. Kroeger, (615) 574-5177

The purpose of the research and development effort is to develop materials information and processing techniques applicable to the production of high $T_c$ oxide superconductors in bulk form with high critical current density. A primary focus of the effort is toward reducing or eliminating grain boundary problems in polycrystalline material. Techniques are developed for the production of high purity, homogeneous, morphologically controlled precursor powder and the fabrication of conducting high-$T_c$ oxides in complex shapes. Efforts are directed at increasing critical current density through control of microstructural features. The orthorhombic superconducting phase of $YBa_2Cu_3O_{7-x}$ has been shown to be thermodynamically unstable to decomposition by an oxidation reaction initiated at grain boundaries and free surfaces. Phase pure, dense $YBa_2Cu_4O_8$ specimens have been prepared by processes involving hot isostatic pressing and elevated oxygen-pressure processing. A jointly sponsored program with STEPS and the Advanced Industrial Materials Program has been initiated to study the processing of thick powder deposits prepared electrophoretically on metallic and ceramic substrates. Heat treatment studies are in progress. Also, a study of the effects of process parameters on the properties of powders produced by aerosol decomposition is nearly complete.

Keywords: Superconductors, Crystal Defects and Grains, Boundaries, Structure, Consolidation of Powders, Powder Synthesis and Characterization

179. Materials Durability in the Zinc/Bromine System — FY 1990 $19,000

DOE Contact: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: C. Arnold, (505) 844-8728

Project efforts are directed toward improving the chemical durability of materials in zinc/bromine battery environments. Sandia has characterized several materials used in zinc/bromine batteries produced by Energy Research Corporation, Johnson Controls, and Toyota. The purpose of characterizing materials is twofold: to obtain baseline data for subsequent battery post-mortem analysis and to detect property variations which may be attributable to non-uniform processing.

Keywords: Batteries, Corrosion

180. Solid-Electrolyte Cell Research — FY 1990 $225,000

DOE Contact: A. Landgrebe, (202) 586-1483
Argonne National Laboratory Contact: C. Christianson, (312) 972-7563

Efforts are directed toward developing glass-to-header seals that are mechanically stable and provide hermetic seals for use in sodium/sulfur cells. The material investigated for this purpose was a sodium-ion conducting glass (in mol%): 42 $Na_2O$, 8 $Al_2O_3$, 5 $ZrO_2$, and 45 $SiO_2$, which has a resistivity of about 220 ohm-cm at 300°C. Ceramics based on magnesium oxide were found to be ideal candidates for sealing the glass to a header.

Keywords: Ceramics, Solid-Electrolytes

181. Zinc Electrode Morphology in Acid Electrolytes

FY 1990
$100,000

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

Zinc electrode morphology is studied in acidic zinc chloride and zinc bromine electrolytes to provide the fundamental information needed to improve the design and performance of zinc/halogen batteries. *In situ* studies of the formation of zincate ions in Zn/AgO cells containing 12 M potassium hydroxide were initiated. Additional studies were made in 12 M KOH with silicate, sorbitol and mixtures of both additives.

Keywords: Electrodes, Morphology

182. Zinc/Air Battery Development for Electric Vehicles

FY 1990
$149,000

DOE Contact: A. Landgrebe, (202) 586-1483
Metal Air Technology Systems International Contact: R. Putt, (404) 876-8203

Demonstrated that zinc loadings greater than 100 $mAh/cm^2$ can be attained in a reticulated electrode structure. A process was developed for pre-plating copper substrate on a reticulated electrode structure. The process yielded a dense, uniform, and continuous zinc deposit.

Keywords: Batteries, Electrode

183. Polymeric Electrolytes for Ambient-Temperature Lithium Batteries

FY 1990
$47,000

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

A detailed study by thermal gravimetric analysis and differential scanning calorimetry of polyethylene oxide was undertaken to determine the effects of hydration/dehydration on parameters such as $T_g$, maximum water uptake, amount of coordinated water, and the reversibility of hydration/dehydration of polymeric electrolytes for lithium batteries. The results show that the hydration/dehydration characteristics of the electrolyte are strongly influenced by the identity of the cation in the electrolyte.

Keywords: Polymers, Batteries

184. Exploratory Cell Research and Study of Fundamental Processes in Solid State Electrochemical Cells

FY 1990
$ 0

DOE Contact: A. Landgrebe, (202) 586-1483
University of Minnesota Contact: W. Smyrl, (612) 625-0717

This study was completed in FY90. The program's objective was to perform research and development to support the development of high-performance rechargeable batteries that are desired for electric vehicles or utility load-leveling systems. The major thrust was investigation of solid-polymer-electrolyte rechargeable cells based on polyethylene oxide (PEO) using Na and divalent metal anodes that are alternatives to Li. Other studies were conducted using polypyrrole (PPY) for the cathode. Differential scanning calorimetry (DSC) and x-ray diffraction studies were conducted on $(NaCF_3SO_3)_xPEO$. PPY was found to be stable in aqueous and oxygen environments. A $Na/NaCF_3SO_3(PEO)_8/PPY$ cell was fabricated using thin-film technology. The cell had an open-circuit voltage of 2.45 V at 100 °C and a theoretical capacity of 22.7 $\mu$Ah. The cell was discharged at a constant current of 7.6 $\mu$A (C/3 rate) to a cell voltage of 1.5 V, and charged at constant current of 7.6 $\mu$A to 3.1 V. The observed capacity was 45 percent of theoretical, and the columbic efficiency was 70 percent for the first cycle. The subsequent four cycles also showed similar performance.

Keywords: Conducting Polymers, Batteries, Thin Films

185. Corrosion, Passivity, and Breakdown of Alloys Used in High-Energy-Density Batteries

FY 1990
$88

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

Over the past year a complete investigation of the passivation behavior of iron in anhydrous propylene carbonate (PC) containing 0.5 M $LiClO_4$ was undertaken. In addition, preliminary studies of the effect of the electrolyte anion on the phenomena observed have been conducted by investigating passivation in the presence of 0.5 M $LiAsF_6$. Recent studies of iron in PC containing 0.5 M $LiAsF_6$ showed that iron pits upon modest anodic polarization, indicating that the air-formed film is not as protective in the presence of $AsF_6^-$ as in the presence of $ClO_4^-$. The reasons for this behavior is the subject of ongoing work.

Keywords: Passivation, Metals: Ferrous, Batteries

186. Advanced Chemistry and Materials for Fuel Cells FY 1990
$100,000

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

Work has focused on investigating oxygen reduction in new acidic electrolytes and evaluating new fuel cell electrocatalysts. A new process was developed for making more uniform, carbon-supported platinum samples. This improved the quality of the EXAFS data. EXAFS studies were carried out on Fe-TMPP on Cabot Black Pearls Carbon.

Keywords: Fuel Cells, Catalysts, Oxygen Reduction

187. Electrocatalysts for Oxygen Reduction and Generation FY 1990
$196,000

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

Both *ex situ* and *in situ* Fourier transform infrared reflectance absorption spectroscopy (FTIRRAS) were used to examine monolayers of adsorbed iron and tetrasulfonated phthalocyanine (CoTSPc) on silver, highly ordered pyrolytic graphite (HOPG), and ordinary pyrolytic graphite (OPG). In addition to nitrogen-containing polymers, other polymers such as polystyrene mixed with cobalt acetate and Vulcan XC-72 carbon and heat-treated at 800 °C were examined.

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

Device or Component Fabrication, Behavior or Testing

188. Processing Methods of HTS Thin Films for Metal Tape Conductors FY 1990
$384,000

DOE Contact: R. Eaton, (202) 586-1506
Lawrence Berkeley Laboratory Contact: N. E. Phillips, (415) 486-4896

Methods are being investigated for producing thin films of high-$T_c$ superconductors with appropriate substrate, buffer, and passivating materials to provide a basis for the fabrication of practical tape conductors. The film deposition techniques under investigation are reactive magnetron sputtering and pulsed laser deposition. Near-term target values for the critical current density are $10^5$ A/cm$^2$ for the film and $10^4$ A/cm$^2$ for the tape conductor (at 35 K and 2 T). The pulsed laser deposition technique was used to produce superconducting YBCO films on buffered metal substrates. Laser deposition processing for Bi-Sr-Ca-Cu-O on MgO substrates (using contained Pb and Sb substituted for Bi) resulted in 2212 phase films deposited successfully without post-annealing. Sputtered YBCO films deposited on YSZ, strontium titanate, or silver exhibited critical temperatures not far below those deposited on single crystals, but critical currents were reduced to bulk levels. Films which showed the most anisotropy in electrical measurements also showed the best c-axis ordering in diffraction measurements. $J_c$ measurements on YBCO films on metal substrates have only shown "bulk-like" values on the order of $10^3$ A/cm $^2$, which decline sharply in the presence of a magnetic field.

Keywords: Superconductors, Coatings and Films, Composites, Chemical Properties

189. Proton-Exchange-Membrane Fuel Cells for Vehicles — FY 1990 $1,300,000

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

Los Alamos National Laboratory conducts three major proton-exchange-membrane (PEM) fuel cell projects. These projects seek to: 1) develop better gas diffusion electrodes, 2) measure and model the mass transport properties and conductivity of proton-conducting membranes, and 3) measure the operating characteristics of single PEM fuel cells and determine the conditions providing optimal performance. In FY 1989, measurements of water drag under experimental conditions close to those of an operating PEM fuel cell were initiated. The profile of Nafion impregnated in Prototech electrodes was evaluated by employing an electron probe microanalyzer. A series of tests were also performed on the effects of ionomeric membrane thickness on the performance of single PEM cells.

Keywords: Fuel Cells, Separators, Electrodes

190. Solid Polymer Electrolytes for Rechargeable Batteries — FY 1990 $97,000

DOE Contact: A. Landgrebe, (202) 586-1483
SRI International Contact: D. MacDonald, (415) 859-3195

High-conductivity polymeric electrolytes for rechargeable lithium cells are developed. In FY 1989, poly(ethyleneimine) and poly(aloxane) based polymers were successfully synthesized.

Keywords: Polymers, Electrolytes, Batteries

191. Advanced Membrane Development for the Zinc/Bromine System

FY 1990
$125,000

DOE Contract: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: C. Arnold, (505) 844-8728

The primary emphasis of this task is to select and evaluate chemical pretreatment techniques for use on the silca-microporous polyethylene separators used in the zinc/bromine battery technology. The effect of impregnating an advanced proprietary separator under development at Johnson Controls, Inc. with a commercial sulfonated polyester obtained from Eastman Kodak is being explored. Initial tests indicate that a superior balance between resistivity and bromine permeation rate was achieved. Radiation grafting experiments were carried out in which methacrylic acid was grafted into the pore structure of an inexpensive separator. To determine the conditions required for effective grafting, a scoping type study was carried out. Experiments are in progress to increase the graft yields in an effort to further reduce the rate of bromine transport.

Keywords: Polymers, Batteries, Composites

192. Improved Chromium Platings for Sodium/Sulfur Containers

FY 1990
$60,000

DOE Contact: A. Landgrebe, (202) 586-1483
Sandia National Laboratory Contact: J. W. Braithwaite, (505) 844-7749

This study focused on the identification of techniques to improve the quality and efficiency of plating chromium onto the inside of sodium/sulfur containers. The initial screening of three potential electroplating methods was completed in FY89 with encouraging results with respect to deposit quality and performance. However, recent analyses showed that conventional chromium electroplating will not be cost effective and possibly not environmentally acceptable. In FY90, two alternative techniques were evaluated that could potentially solve these problems: (1) electroless chromium plating, and (2) electrolytic plating using trivalent chromium. Poor quality eliminated electroless plating, and inadequate corrosion protection was provided with the trivalent chromium. This activity will not be continued in FY91.

Keywords: Batteries, Corrosion, Electrolytes

# OFFICE OF ENERGY RESEARCH

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

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

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

- Office of Basic Energy Sciences: Division of Engineering and Geosciences; Division of Materials Sciences; Division of Advanced Energy Projects
- Office of Health and Environmental Research: Division of Physical and Technologies Research
- Office of Fusion Energy
- Small Business Innovation Research Program

## Office of Basic Energy Sciences

### Division of Materials Sciences

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

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

There are three subprograms:

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

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

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

The operating funds for FY 1990 for the Division of Materials Sciences were $198,400,000. This was allocated to 434 projects. Many projects cross the traditional categories and, for example, involve property-structure relationships. Nevertheless, the approximate funding distribution for FY 1990 was:

| | $ (Millions) |
|---|---|
| Materials Preparation, Synthesis, Deposition, Growth or Forming | 21.5 |
| Materials Structure and Composition | 28.6 |
| Materials Properties, Behavior, Characterization or Testing | 84.1 |
| Device or Component Fabrication, Behavior or Testing | -- |
| Facilities | 64.2 |

The DOE contact for this Division is Iran Thomas, (301) 353-3427. For specific detailed information, the reader is referred to DOE publication Materials Sciences Programs Fiscal Year 1990 (DOE/ER-0483P dated January 1991). This publication contains: summaries of all funded programs at DOE laboratories; summaries of all funded grant programs in universities and private sector organizations; summaries of all Small Business Innovation Research programs; major user facilities (descriptive information); other user facilities; cross-cutting indices: investigators, materials, techniques, phenomena, environment. Limited copies may be obtained by calling (301) 353-3427.

Division of Engineering and Geosciences

Materials research in the Division of Engineering and Geosciences is sponsored by two different research programs, as described below.

The BES Engineering Research Program was started in 1979 to help resolve the numerous serious engineering issues arising from efforts to meet U.S. energy needs. The program supports fundamental research on broad, generic topics in energy related engineering topics not as narrowly scoped as those addressed by the shorter term engineering research projects sponsored by the various DOE technology programs. Special emphasis is placed on projects which, if successfully concluded, will benefit more than one energy technology.

The broad goals of the BES Engineering Research Program are: (1) To extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and (2) To broaden the technical and conceptual base for solving future engineering problems in the energy technologies. The DOE contact for this Program is Oscar P. Manley, (301) 353-5822.

The BES Geosciences Research Program supports research that is fundamental in nature and of long-term relevance to one or more energy technologies, national security, energy conservation, or the safety objectives of tl , Department of Energy. It is also concerned with the extraction and utilization of such resources in an environmentally acceptable way. The purpose of this program is to develop geoscience or geosciences-related information relevant to one or more of these Department of Energy objectives or to develop the broad, basic understanding of geoscientific materials and processes necessary for the attainment of long-term Department of Energy goals. In general, individual research efforts supported by this program may involve elements of several different energy objectives. The DOE contact for this Program is William C. Luth, (301) 353-5822.

Materials Properties, Behavior, Characterization or Testing

193. New Ultrasonic Imaging and Measurement Techniques for NDE FY 1990 $254,388

DOE Contact: Oscar P. Manley, (301) 353-5822
Ames Laboratory, Iowa State University Contact: D. O. Thompson, (515) 294-5320

The objective of this project is to develop new knowledge and techniques for the nondestructive detection and characterization of flaws and nondestructive measurements of material properties that are of importance in obtaining reliability and integrity. In order to achieve this goal, efforts are made to develop new and novel ultrasonic NDE capabilities and to characterize emerging materials. Use is made of a multiviewing system previously developed in this work and quantitative elastic wave theories in the interpretation of results as well as microfocus radiography and eddy current techniques. Three major thrusts are being pursued:

1. Nondestructive material characterization methods are being explored for high transition temperature superconducting ceramics using three types of probing fields: X-ray, eddy current, and ultrasound. Efforts are aimed at nondestructive measurements that can be used to monitor material processing techniques.

2. Novel techniques have been developed that allow the fabrication of ultrasonic transducers that have fundamentally important wave propagation properties of engineering significance. Two such transducers, a Gaussian beam transducer and a Bessel beam transducer, have been developed. The Gaussian beam is particularly desirable for inspection in the near field and the Bessel beam can potentially lead to diffraction-free elastic waves.

3. New techniques for ultrasonic computed tomographic imaging (reconstruction) are being explored that utilize elastic wave scattering models and the multiviewing instrumentation. This is an important innovation in that images so obtained are expected to be free of distortions due to effects of material anisotropy and complex surfaces encountered in some current imaging techniques.

Keywords: Nondestructive Evaluation, Ultrasonic, Fracture

194. <u>Bounds on Dynamic Plastic Deformation</u> FY 1990
$127,194

DOE Contact: Oscar P. Manley, (301) 353-5822
Argonne National Laboratory Contact: C. K. Youngdahl, (312) 972-6149

Analytical studies are being performed to develop load correlation parameters which can be used in approximating or bounding the dynamic plastic deformation of structures. In many applications where the load is transmitted to the structure through a fluid, details of the load history and spatial distribution significantly affect the final plastic deformation. The objective of the program is to devise load correlation parameters based on various weighted integrals of the time-space load distributions which can be used to characterize the effects of the load without resorting to detailed numerical analysis. These load correlation parameters have three important uses: to perform design and safety analyses of structures over a wide range of design variables and loadings; to validate computer programs which have a nonlinear dynamic plasticity capability; and to correlate experimental simulations with actual or predicted events. The dynamic plastic deformation of some basic structural configurations will be analyzed for loadings which vary both in magnitude and region of application with time. Load correlation parameters will be hypothesized and their usefulness in predicting final plastic deformation will be determined. The analyses will be based initially on a rigid, perfectly plastic material model and small deformation response, but will be extended to include strain hardening, and initial elastic response period, and large deformation interactions.

Keywords: Plastic Deformation

195. <u>Continuous Damage Theory</u> FY 1990
$53,000

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The efforts in the first two years of this research program were focused on the development of a micromechanically inspired continuum damage mechanics model. Specifically, the objective was to formulate a rigorous micro-to-macro transition along with the conditions which must be satisfied for this transition to be valid. For example, it was demonstrated that the change in elastic compliance is ia proper choice for the thermodynamic macro-flux since it represents an orientation weighted volume average of micro-fluxes. The corresponding affinity is the energy release rate integrated along the crack perimeter and averaged across its surface. The macro-potential is subsequently determined as an inner envelope of the micro-potential. The corresponding damage surface is a convex piecewise smooth hypersurface possessing the normality property. The ensuring computations clearly indicate the simplicity and accuracy of the proposed model in several illustrative examples.

The micro-to-macro transition is, however, proven to be valid only as long as the application of the effective continual theories is justified. In other words, the macro flow potential cannot be proven to exist when the influence of the direct interaction of micro-defects on the deformation becomes significant.

One of the most important aspects of the analyses of brittle deformation processes is the determination of failure which is, obviously, associated with a critical microcrack density. However, the analytical modeling of the so-called cooperative phenomena, characterized in the considered case by a disorder of the material microstructure and the interaction of many defects of random geometry, distribution and orientation represents a serious problem. This class of problems, being inherently nondeterministic in nature, is seldom if ever addressed in continuum mechanics. A promising strategy, to be explored in the continuation of this research program, is to consider the application of the so-called percolation theory. One of the two main problems is to make a transition between the lattice and continuum percolation theory and recover the damage micro-flux (Budiansky-O'Connell variable) and enable mapping between the two models. The other problem is that the disorder is introduced into the percolation model traditionally by a bimodal distribution which might be too restrictive for real materials having a richer hierarchy of strengths on the micro-scale. Nevertheless, it is felt that the percolation theory offers a viable framework for the studies of the brittle deformation processes in the vicinity of the percolation thresholds (which are different than those associated with transport phenomena). The application of the percolation theory is important since it enables studies of estimates which the local fluctuations of stresses (hot-spots) and strengths (weak-links) have on the failure of the material.

Keywords: Metals: Ferrous, Fracture, Fatigue, Creep

196. Transport in Porous/Disordered Materials — FY 1990 $66,650

DOE Contact: Oscar P. Manley, (301) 353-5822
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The aim of this project is the construction of theories of the transport processes-diffusion, fluid flow, electromagnetic wave propagation, etc., in materials where strong interactions or disorder cause a near stoppage of the transport. Of special interest are materials with percolation thresholds, where the disorder blocks transport altogether, and systems near a glass transition. The research is broadly based and a wide range of theoretical and computational techniques are employed. Progress along three fronts was made in the past year.

Harmonic normal mode analysis is routinely applied to stable solids, but it is not normally considered useful for fluids. We have developed a new method for fluid dynamics, based upon normal mode analysis, in which transport is governed by the unstable modes of the system. The method worked extremely well for supercooled liquids and is now being applied to suspensions of spheres.

Glass ceramics are composed of irregular crystallites in a glassy matrix. The propagation of light through these disordered materials was studied. The structure of the crystallites was related to the properties of the scattered light in a completely new scheme which requires the intensity statistics, but no knowledge of optical properties.

High intensity light will break chemical bonds and cut material. A fairly comprehensive model of this very nonlinear process was constructed and solved, with qualitative agreement with several observations. Computer simulation of the phenomenon was begun, with an eye to the study of laser-induced shock waves and to sorting out the "energy bookkeeping," the ultimate destinations of the laser energy.

Keywords: Porous/Disordered Media, Transport

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

<u>FY 1990</u>
$47,804

DOE Contact: Oscar P. Manley, (301) 353-5822
University of Connecticut Contact: E. H. Jordan, (203) 486-2371

The goal of this research is the development and verification of a model of the time and history dependent viscoplastic deformation behavior of polycrystalline metals. Single grain behavior has been derived by summing postulated slip behavior on crystallographic slip systems. Multi-grain behavior will be obtained by summing deformation occurring in different grains while accounting for grain interaction through a self-consistent micromechanics approach. The model will also represent grain boundary sliding through the use of a solution recently published by T. Mura.

High temperature experiments on Hastelloy-X will be used to verify the model. Since crystal properties used for input to the model are currently being determined. Using these properties the behavior of polycrystal Hastelloy-X will be predicted and then compared with polycrystalline experiments recently completed. Prediction of these tests constitute a critical test for the theory.

The model will not only predict the viscoplastic response of polycrystals but also will allow metallurgical findings usually stated in crystallographic terms to be more directly incorporated into the model. The explicit calculation of grain boundary sliding will help illuminate the role played by grain boundary sliding in the overall deformation during complex load histories. Grain boundary sliding deformation plays an important role in material damage and the model should be useful in life prediction under complex variable temperature conditions.

At present, the single crystal model is available and the self-consistent model without grain boundary sliding has been derived and is being programmed.

This work is being done with the cooperation of Engineering Science Software, Inc., working under a related contract. Single crystal specimens have been provided by Pratt and Whitney, Inc.

Keywords: Micromechanical, Viscoplasticity, Grain Boundary, Crystallographic Slip, High Temperature, Experiments

198. A Micromechanical Viscoplastic Stress-Strain Model with Grain Boundary Sliding

FY 1990
$46,048

DOE Contact: Oscar P. Manley, (301) 353-5822
Engineering Science Software, Inc., Contact: K. P. Walker, (401) 231-3182

The aim of the project is to develop a viscoplastic constitutive model, with accompanying FORTRAN software, to model the deformation behavior of polycrystalline metals comprised of an aggregate of fcc single crystal grains whose crystallographic axes are oriented at random. The single crystal grains are assumed to be spherical and are modeled with an anisotropic viscoplastic theory based on crystallographic slip along the octahedral and cube slip directions of the fcc metal. The overall response of the polycrystalline aggregate is assumed to be isotropic and is deduced from the single crystal response by means of a self-consistent method. The effect of grain boundary sliding between the grains is being modeled in the self-consistent formulation to assess the importance of including this mechanism in the overall response of the polycrystalline material.

Experimental tests on single crystal specimens of the superalloy Hastelloy-X are being run at the University of Connecticut to determine the material constants in the single crystal constitutive model. The overall response of the self-consistent model of the polycrystalline aggregate will then be theoretically determined and compared with experimental results from isotropic specimens of polycrystalline Hastelloy-X.

The FORTRAN software will allow metallurgical and micromechanical work reported in the literature to be easily embedded in a constitutive (stress-strain) framework for analyzing the overall deformation response of polycrystalline metal aggregates under thermomechanical loading conditions.

Keywords: Micromechanical, Viscoplasticity, Grain Boundary, Crystallographic Slip, High Temperature, Constitutive Model

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

FY 1990
$182,137

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. A measurement technique for simultaneously obtaining particle size, velocity and temperature has been developed. Particle size and velocity are obtained from a dual color combination laser Doppler velocimeter (LDV) and laser particle sizing system. The LDV system consists of a crossed beam technique while particle size is determined from the absolute magnitude of scattered laser light. The particle temperature is determined by a two color pyrometer technique. The spatial resolution is better than $1mm^3$ and allows the distribution of particle size, velocity and temperature to be mapped over laboratory scale flow fields. The influence of particle size, injection rate, torch power, etc., are currently being examined in typical flow fields.

The project is one of six projects comprising a collaborative research program with the Massachusetts Institute of Technology.

Keywords: Plasma Processing, Particle/Plasma Interaction

200. Plasma-Particle Interactions

FY 1990
$568,805

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contacts: C. B. Shaw, (208) 526-8818, S. C. Snyder, (208) 526-1507 and L. D. Reynolds, (208) 526-8335

Plasma processing of materials saves energy and strategic materials, compared to other methods. The high temperatures and temperature gradients unique to plasmas make possible the synthesis or destruction of compounds not achievable by other means. However, for American industry to put this plasma technology to practical use, and thereby improve its competitive position in world markets, it is necessary to minimize the expensive trial and error scale-up from laboratory demonstration through pilot plant experimentation to full production. This goal requires creation of a rational basis for plasma torch design and operation, namely, a set of computer models (being developed at the INEL and at MIT) which have been fully validated by comparison of their predictions with experimental results of diagnostic measurements. The role of this task is to develop the necessary diagnostic methods, make the test results available to the modelers, and jointly determine what further features are needed in both the models and the diagnostics.

While a half dozen diagnostic methods have been developed and tested in this task, in FY 1990 attention centered as (1) a suite of emission spectroscopy measurements, interpreted by the generalized multi-temperature equilibrium model, to determine the significance of departure of thermal plasmas from the commonly assumed local thermal equilibrium; and (2) high resultion absolute intensity measurement of Doppler broadened and Doppler shifted laser radiation Rayleigh scattered by the atoms and ions of the plasma. The latter permits simultaneous determination of the true kinetic temperature, local mean flow velocity, and density of the scatterers.

Keywords: Plasma Processing, Diagnostics, Computer Model

201. Modeling of Thermal Plasma Processes | FY 1990 $ 0

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contacts: J. D. Ramshaw, (208) 526-9240 and C. H. Chang, (208) 526-2886

Optimization of thermal plasma processing techniques requires a better understanding of the space- and time-resolved flow and temperature distributions in the plasma plume and of the interaction between the plasma and a particulate phase. This research is directed toward the development of a comprehensive computational model of thermal plasma processes and plasma-particle interactions capable of providing such information. The model is embodied in the LAVA computer code for two- or three-dimensional transient or steady state thermal plasma simulations. LAVA uses a rectangular mesh with an excluded volume function to represent geometrical obstructions and volume displaced by particles. Simple highly vectorizable numerics are utilized, with rapid steady state and low-speed flow options. The plasma is represented as a multicomponent fluid governed by the transient compressible Navier-Stokes equations. Real gas physics is allowed for by temperature-dependent specific heats and transport properties. Multicomponent diffusion is calculated in a self-consistent effective binary diffusion approximation, including ambipolar diffusion of charged species. Both k-epsilon and subgrid-scale turbulence models are included. Dissociation, ionization, and plasma chemistry are represented by means of general kinetic and equilibrium chemistry routines. Discrete particles interacting with the plasma will be represented by a stochastic particle model similar to that previously used to model liquid sprays. This model allows for spectra of particle sizes, shapes, temperatures, etc., thereby capturing the important statistical aspects of the problem. It will include sub-models for the various plasma-particle and particle-particle interaction processes, including melting, evaporation, condensation, nucleation, agglomeration, and coalescence.

Keywords: Plasma Processing, Optimization, Computational Model

202. Nondestructive Evaluation of Superconductors | FY 1990 $177,371

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contact: K. L. Telschow, (208) 526-1264

The purpose of this task is to perform fundamental research which will lead to the development and application of new nondestructive evaluation (NDE) techniques and devices for the characterization of high-temperature superconducting materials. In the near future, application of these new superconductors will require NDE methods for evaluating the properties of wires, tapes and coatings. Microstructural and, particularly, superconducting properties, must be measured noninvasively in a manner capable of providing spatial information so that fabrication processes can be optimized. Although the fabrication of these ceramic materials is being pursued by many different techniques at present, there is enough similarity in the different superconducting materials and the fabricated forms to begin research into NDE measurement techniques. In FY89 this project began identifying techniques that can determine critical superconducting properties on a local scale. This has resulted in the use of AC induced currents in conjunction with DC transport currents to determine critical currents and dissipation locally. The analysis of these measurements is being carried out with the aid of the London and "Critical State" models for supercurrent flow in these materials. These results are being correlated with material microstructure information and other measurement techniques.

Keywords: NDE, Superconductors

203. Intelligent Control of Thermal Processes | FY 1990 $480,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contacts: H. B. Smartt, (208) 256-8333 and J. A. Johnson, (208) 526-9021

This project addresses intelligent control of thermal processes as applied to materials processing. Intelligent control is defined as the combined application of process modeling, sensing, artificial intelligence, and control theory to process control. The intent of intelligent control is to produce a good product without relying on post-process inspection and statistical quality control procedures. The gas metal arc welding process is used as a model system;

considerable fundamental information on the process has been developed at INEL and MIT during the past six years. Research is being conducted on an extension of the fundamental process physics, application of neural network-like dynamic controllers and signal/image processors, and development of noncontact sensing techniques. Tasks include physics of nonlinear aspects of molten metal droplet formation, transfer, and substrate thermal interaction; understanding the relationship of neural network structure and associated learning algorithm to model development and learning dynamics in neural networks with the objective of obtaining a fundamental understanding of network transfer functions; and advanced sensing, including the propagation and interaction of ultrasound in metallic solid and liquid media.

This project is part of a collaborative research program with the Massachusetts Institute of Technology.

Keywords: Thermal Processes, Intelligence Control

204. Elastic-Plastic Fracture Analysis Emphasis on Surface Flaws — FY 1990 $385,706

DOE Contact: Oscar P. Manley, (301) 353-5822
Idaho National Engineering Laboratory Contact: W. G. Reuter, (208) 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 for comparisons with data developed from specimens containing surface cracks.

These comparisons are presently underway for 6.4 and 12.7 mm thick surface-flawed specimens. Metallographic techniques are being used to measure crack tip opening displacement and remaining ligament configurations for comparison with analytical models. Other techniques including microphotography and replicating of the crack tip region to complement the above measurements are being used to identify limits and capabilities of each technique. Moire interferometry techniques are being used to evaluate and quantify the deformation in the crack region. These data are being used to experimentally measure J and CTOD for standard (CT and SENB) specimens as well as for specimens containing surface cracks. The above tests have been supplemented by using specimens fabricated from aluminum (dimple rupture only) and titanium. The titanium specimens are being used to study the fracture behavior and the ability of existing models to predict failure for weldments. Moire interferometry techniques are being used to study the local constitutive behavior and the fracture process at the crack tip region of the weldment. Automated techniques are being developed to obtain, store and analyze the moire data.

Keywords: Fracture, Surface Flaws, Elastic-Plastic

205. Heat Transfer to Aqueous Polymer Solutions

FY 1990
$70,144

DOE Contact: Oscar P. Manley, (301) 353-5822
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The goal of the research is to study the fluid mechanical and heat transfer behavior of viscoelastic aqueous polymer solutions. The ultimate objective is to provide a basis for predicting the performance of such fluids. At the present time, two basic investigations are underway:

a. Pool boiling behavior of aqueous solutions of several high molecular weight polymers, including hydroxyethyl cellulose, carboxymethyl cellulose (CMC) and polyacrylamide and a comparison with pool boiling performance of deionized water.

b. Forced convection behavior of viscoelastic fluids in laminar flow through rectangular channels.

To date the following results have been found:

a. High concentrations of the aqueous hydroxyethyl cellulose solutions yield higher values of the boiling heat flux than found with deionized water when compared at the same wall-to-fluid temperature difference. In contrast, aqueous polyacrylamide solutions yield lower values of boiling heat flux than found with deionized water when compared at the same wall-to-fluid temperature. A new series of measurements with another cellulose (CMC) is underway to determine if this family of polymers has special boiling properties. Detailed rheological properties are being measured to provide some insight into the boiling behavior.

b. The forced convection heat transfer performance of viscoelastic fluids in laminar flow through rectangular channels is considerably higher than predicted for purely viscous fluids, although the measured friction factor is in good agreement with the value predicted by the purely viscous analysis. Measurements of the dynamic properties including phase shift under oscillatory condition are shown to be related to observed heat transfer behavior.

Keywords: Heat Transfer, Aqueous Polymer Solutions

206. Pulse Propagation in Inhomogeneous Optical Fibers FY 1990
$76,091

DOE Contact: Oscar P. Manley, (301) 353-5822
University of Maryland Contact: C. Menyuk, (301) 455-3501

Many systems, such as computers, sensors for intelligent machines, and high resolution graphics require ever increasing channel capacity to transfer information from one part of the system to another. Recent developments have shown that fiber optics offer a suitable medium to accommodate the growing need for large data rates. This is of particular concern to energy systems using this transmission medium because the presence of radiation and of other effects which may affect the integrity of essential communication links in those systems.

This research will study the effects of slowly varying inhomogeneities and localized imperfections in the fibers on their transmission properties.

Three topics are of particular interest:

1. *Behavior near the zero dispersion point.* This point denotes the frequency at which the wave propagation speed is independent of the wavelength—a point preferred for operating at the highest possible data rates because of the lowest power needs. The actual zero dispersion point depends on the material properties as well as on the geometry of the fiber. Small random variations in those properties along the length of the fiber will have a destructive effect on the integrity of the signal propagated by the fiber. At present it is not known how much of a limiting factor that is for a given statistical distribution of the slowly varying inhomogeneities.

2. *Effects of a varying birefringence.* As the material properties in the fiber change from point to point so does the fiber's response to the polarization of the electromagnetic wave. Under certain conditions that polarization may be changed enough by mixing to affect the properties of the transmitted signal. Again, while something is known about the effects of a single polarization mixing event on a pulse in the fiber, nothing is known about the effects of many such events and how they can be related to the properties of the fiber.

3. *Bubbles and inclusions in optical fibers.* Because such imperfections often focus the incident electromagnetic beam they are known to cause damage to the fiber itself. Previous studies have not taken into account the so-called ponderomotive forces, that is body forces arising from the interactions of the gradients in the properties of the fiber material with the incident electromagnetic fields.

This research will address the three topics enumerated above, first in the linear regime and then in the non-linear regime. While this effort is primarily theoretical, it will benefit from close ties to related experimental work at Bell Labs, at NRL and at FDA.

Keywords: Optical Fibers, Pulse Propagation, Inhomogeneities, Imperfections

207. High-Temperature Gas-Particle Reactions

FY 1990
$123,110

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contacts: J. F. Eliott, (617) 253-3305 and P. P. Bolsaitis, (617) 253-5069

The purpose of the research program is to examine the physico-chemical behavior of individual inorganic particles in conditions simulating those to which particles are exposed during thermal plasma processing. The particle is suspended in a closed chamber by an electrostatic field, and it is heated by a pulsed laser beam. The composition of the gas in the reactor can be controlled, and the temperature of the particle can be measured with a time resolution as short as two-tenths to one millisecond. Equipment for optical imaging of the particle during processing is being developed.

Study is in progress of melting, vaporization, and solidification of particles of ceramic materials (alumina, zirconia), metals (Al-Ni alloys, aluminum), and carbides (silicon carbide, WC-Co, and hard facing materials). Methods and procedures for improving the accuracy of single- and two-color temperature measurements during rapid heating and cooling of the particles have been developed. Measurements have been made of the evaporation of oxide particles while they are heated and cooled.

This work is closely connected with the experimental program on plasma processing at the Idaho National Engineering Laboratory, and other plasma processing studies in the Department of Materials Science and Engineering at MIT. The combination of data from this investigation, the data base from INEL on plasma spraying, and results of modeling of plasma spraying by Professor Szekely's group (MIT) will provide much more complete understanding of plasma processing of materials than has been available heretofore.

Keywords: Plasma/Particle Interaction

208. Mathematical Modeling of Transport Phenomena in Plasma Systems FY 1990
$92,806

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 heat flow, fluid flow and mass transfer phenomena in thermal plasma systems and to compare the theoretical predictions with experimental measurements.

A general formulation of the problem has been developed and an extensive set of computed results has been generated, describing the velocity profiles, temperature profiles and concentration profiles in a variety of non-transferred arc systems. The theoretical prediction were found to be in good agreement with measurements reported by researchers at the Idaho National Engineering Laboratory and in two university laboratories. More recent work is concentrating on plasma-particle interactions and on transport phenomena inside plasma torches. This latter work is very promising in providing a rational science base for plasma torch design.

Keywords: Plasma Systems, Transport Properties

209. Multivariable Control of the Gas-Metal Arc Welding Process FY 1990
$152,467

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: David E. Hardt, (617) 253-2429

The Gas Metal Arc Welding Process (GMAW) is a highly productive means for joining metals, and is being used increasingly for structures and pressure vessels. It presents a challenging multivariable control problem entailing both geometric and thermal outputs. These outputs all combine to determine the strength and toughness of the resulting joint. The overall objective of this work is to examine the problem of simultaneous regulation of all real-time attributes of a weld. Past work has established the viability of independent control of thermal characteristics, and the present work is examining the geometric aspects of weld pool control.

One objective of this work is to develop basic process modeling and control schemes to allow independent regulation of the weld bead width and height.

A control model relating wirefeed and travel speed to width and height was developed using transfer function identification techniques applied to a series of step welding tests. The resulting discrete transfer function was found to be non-linear in both the static and dynamic parts, owing to a strong dependence upon the input magnitudes. This model was then used to develop a decoupling controller design that cancels the non-linear behavior using gain scheduling. Proper regulation of the process was demonstrated, but the limited range of control afforded by this process, and the significant process delays that were in evidence, led to very poor disturbance rejection. It is apparent that the GMAW process will need significant modifications to overcome these problems. In an attempt to merge previous results on the regulation of thermal characteristics in real-time with the geometry control work, we are developing a control system to independently regulate the weld bead width and the width of the heat affected zone (HAZ). Initial work is concentrating on simulation of wide seam welding using an analytical heat transfer model as well as a finite difference process model. A key issue in the problem is the strong coupling between the inputs (current and travel speed) and the outputs. The use of high frequency transverse motion of the torch is being investigated as a means of overcoming this coupling. Once the control latitude is increased, a two variable control scheme based on both video and infra-red sensing will be implemented.

Finally, the depth of penetration of a weld is the most important indicator of weld strength, yet it is the one variable that is essentially impossible to measure directly. A real-time depth estimator has been developed based on the solution of an inverse heat transfer problem. Surface temperature measurements match the predicted values. Initial experiments with this model, using surface temperature measurements from the top and bottom of the weld, have shown accurate and rapid convergence, and development of a depth control system based on this estimator is now proceeding.

Keywords: Welding, Control

210. <u>Metal Transfer in Gas-Metal Arc Welding</u> <u>FY 1990</u> $124,057

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contact: T. W. Eagar, (617) 253-3229

The present research is part of a cooperative program among faculty at MIT and staff at Idaho National Engineering Laboratory to develop sensing and control methods which can be used to automate the gas-metal arc welding processes.

Current research emphasizes understanding of the forces controlling droplet detachment in gas-metal arc welding. Experimentally, a laser back lit viewing system has been developed which permits viewing of anode and cathode jet phenomena. Welds have been made with a variety of different shielding gases (argon, helium, carbon dioxide). It is seen that the anode spot behavior changes dramatically with changes in both metal and gas composition.

This experimental information is being coupled with a model of the forces controlling metal transfer. These include gravitation, surface tension, aerodynamic drag, electromagnetic (Lorentz) force and plasma jet momentum. Initial studies show that globular transfer can be described quantitatively by previous theories which were presented originally in only a qualitative manner. Quantification of previous explanations of spray transfer depart markedly from the experimental observations. A new model of the globular to spray transition has been hypothesized and is currently being studied with a finite element model.

It is believed that this work will ultimately be useful in understanding metal transfer in pulsed current gas metal arc welding. This study also interfaces with the experimental and theoretical gas metal arc welding control models being developed at MIT by Professor D. Hardt and at INEL.

Keywords: Welding, Control

211. Modeling and Analysis of Surface Cracks | FY 1990 $188,453

DOE Contact: Oscar P. Manley, (301) 353-5822
MIT Contacts: David M. Parks, (617) 253-0033 and F. A. McClintock, (617) 253-2219

This research focuses on the analysis of ductile crack initiation, growth and instability in part-through surface-cracked plates and shells. The overall approach consists of careful calculations of crack front stress and deformation fields, and correlation of cracking with experimental observations being conducted at the Idaho National Engineering Laboratory.

Recently, significant progress has been achieved in developing and applying a two-parameter description of crack front fields. The amplitude of crack tip deformation is characterized by J or CTOD, while the hydrostatis constraint in the near-tip region correlates well with a parameter related to the so-called T-stress, or second elastic Williams' eigenfunction.

Simplified engineering applications of surface crack analysis are being developed in the context of the line-spring model. Specific enhancements include improved elastic-plastic procedures for the practically important case of shallow surface cracks, as well as simple methods for calculating the T-stress along surface cracks fronts.

Keywords: Fracture

212. Thermal Plasma Processing of Materials | FY 1990 $129,723

DOE Contact: Oscar P. Manley, (301) 353-5822
University of Minnesota Contact: E. Pfender, (612) 625-6012

For measuring temperature and velocity fields in plasma systems used for thermal plasma processing, enthalpy probes have been developed and tested in this laboratory. The validity of measured enthalpy and velocity profiles has been checked by performing energy and mass flux balances in an argon plasma jet operated in argon atmosphere.

Ceramic powders of carbides, aluminum nitride, oxides, solid solutions, magnetic and non-magnetic spinels, superconductors, and composites have been successfully synthesized in a Triple DC Torch Plasma Jet Reactor (TTPR) and in a single DC Plasma Jet Reactor. All the ceramic powders with the except of AlN were synthesized using a novel liquid injection method developed to overcome the problems associated with solid injection, in particular for the single DC plasma jet reactor, and to realize the benefits of gas phase reactions.

Equilibrium calculations based on the standard technique of minimization of the system total Gibbs free energy are not adequate for predicting the yield and the proper composition of the products from thermal plasma systems. This is due to domination by nucleation kinetics, a non-equilibrium effect. Therefore, total Gibbs free energy minimization calculations using a quasi-equilibrium modification have been applied to, for example, AlN, ZrC and $MgAl_2O_4$ reactions. The modeling results agree well with experimental data in terms of product yield and composition.

Keywords: Plasma Processing, Plasma Diagnostics

213. Thermophysical Property Measurements in Fluid Mixtures — FY 1990 $509,486

DOE Contact: Oscar P. Manley, (301) 353-5822
National Institute of Standards and Technology Contact: R. Kayser, (301) 975-2483 and J. M. H Sengers, (301) 975-2463

The project aims at the development of accurate measurement capabilities for the thermophysical properties of complex, multiphase, fluid mixtures containing hydrocarbons. The research is being done jointly by two research groups within the Thermophysics Division of the NIST Center for Chemical Engineering. One group is located at the Gaithersburg, MD laboratories and the other at the Boulder, CO laboratories. The properties involved are PVT (pressure-volume-temperature), PVTx (pressure-volume-composition), phase equilibria (liquid-vapor and liquid-liquid equilibria), phase behavior in interfaces, and transport properties (viscosity, thermal conductivity, and diffusion coefficient). The apparatus will be designed for use in corrosive, highly corrosive, and sometimes toxic and flammable fluids with measurements extending to high temperatures (800K) and high pressure (30 MPa and, in some cases, 70 MPa). Also under study are methods for evaluating supercritical solvent mixtures and related fluid mixtures.

The most recently completed apparatus include a variable volume vapor-liquid equilibrium apparatus for moderate temperature ranges; a Langmuir film balance for use with aqueous, hydrocarbon, and biopolymer systems; a magnetic suspension densimeter for high temperatures and pressures; a torsional crystal viscometer for high temperatures and pressures; and a transient hot-wire apparatus for thermal conductivity measurements at high temperatures. The latter two apparatus are capable of reaching pressures near 70 MPa.

Keywords: Thermophysical Properties, Mixtures, Fluids, High Temperature, High Pressure

214. Low Resistivity Ohmic Contacts Between Semiconductors and High-$T_c$ Superconductors

FY 1990
$94,700

DOE Contact: Oscar P. Manley, (301) 353-5822
National Institute of Standards and Technology Contacts: J. Moreland, (303) 497-3641 and J. W. Ekin, (303) 497-5448

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

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

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

215. Transport Properties of Disordered Porous Media from the Microstructure

FY 1990
$91,859

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. The focus is on studying the effect of: porosity, spatial distribution of the phase elements, interfacial surface statistics, anisotropy, and size distribution of the phase elements, on the effective properties of models of both unconsolidated media (e.g., soils and packed beds of discrete particles) and consolidated media (e.g., sandstones and sintered materials).

Both theoretical and computer-simulation techniques have been employed to quantitatively characterize the microstructure and compute the transport properties of disordered media. Statistical-mechanical theory has been used to obtain n-point distribution functions and to study percolation phenomena in continuum random-media models. This has led to accurate predictions of transport properties of realistic models of isotropic as well as anisotropic heterogeneous media. An efficient computer-simulation methodology has been developed to exactly yield effective transport properties in which the transport process is governed by a steady-state diffusion equation. Hence, the algorithm, which is based upon simulating the Brownian motion of a diffusing particle, can be applied to determine the conductivity, dielectric constant, magnetic permeability, diffusion coefficient, and the trapping rate associated with diffusion-controlled reactions among sinks.

Keywords: Disordered Media

216. Effects of Crack Geometry and Near-Crack Materials Behavior on Scattering of Ultrasonic Waves for QNDE Applications — FY 1990 $80,921

DOE Contact: Oscar P. Manley, (301) 353-5822
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A crack in a solid body can, in principle, be detected and characterized by its effect on an incident pulse of ultrasonic wave motion.

The work on this project is concerned with applications of the scattered field approach to the detection and characterization of cracklike flaws. The work is both analytical and numerical in nature. Several forward solutions to model problems have proven to be very helpful in the design of experimental configurations. They are also valuable in interpreting scattering data for the inverse problem.

The efficacy of ultrasonic methods to detect and characterize a crack depends on topographical features of the crack faces, the presence of inhomogeneities in the crack's environment, and on the mechanical properties in the near-crack region. In this work the effects on the scattered ultrasonic field of various features of fatigue and stress corrosion cracks, such as partial crack closure, the presence of microcracks and microvoids, and near-tip zones of different mechanical properties have been investigated. Most of the results have been obtained by formulating a set of singular integral equations for the fields on the boundaries of the scattering obstacles. These equations have been solved numerically by the boundary element method, and the scattered fields have subsequently been obtained by using representation integrals.

For the configuration examined in this paper, crack closure has the most significant effect on far-field scattering.

Keywords: Nondestructive Evaluation, QNDE

217. Inelastic Deformation and Damage at High Temperature | FY 1990 $122,541

DOE Contact: Oscar P. Manley, (301) 353-5822
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A combined theoretical and experimental investigation is performed to study the biaxial deformation and failure behavior of AISI Type 304 Stainless Steel under low-cycle fatigue conditions at elevated temperature. The purpose is to characterize the material behavior in mathematical equations which are ultimately intended for use in inelastic stress analysis and life prediction. Creep-fatigue interaction and ratcheting are of special concern. The long-term goal is the development of a finite element program that can directly calculate the life-to-crack initiation of a component under a given load history.

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 are available together with a reversing direct current potential drop facility. It is intended for early monitoring of damage during cyclic loading. It has been tested out at room temperature.

Uniaxial and torsional ratcheting experiments showed considerable strain accumulation at room temperature and they demonstrate that ratcheting is due to viscous effects. Surprisingly, insignificant ratcheting and rate sensitivity were observed at 550, 600 and 650 °C for uniaxial tests. This unexpected finding was attributed to strain aging in the stainless steel. A finite deformation theory of viscoplasticity based on overstress (VBO) is being developed and is being implemented into a finite element computer program. To simulate the complex hardening behavior of AISI Type 304 Stainless Steel during non-proportional loading, new hardening rules are under investigation and are being implemented into the small deformation VBO theory developed previously.

Keywords: Fracture, Damage

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

FY 1990
$63,594

DOE Contact: Oscar P. Manley, (301) 353-5822
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The motion of vortex structures, in response to applied currents, is a major source of resistance in superconducting networks in magnetic fields. Systems of interest include regular Josephson junction arrays and type II superconductors, such as the new granular high $T_c$ ceramics. Numerical simulations of finite temperature, current carrying networks will be carried out to provide a characterization of vortex response in non-equilibrium situations. For periodic networks, current-voltage (I-V) characteristics will be computed and compared with experimental results. The effects on resistivity of transitions from pinned to unpinned or to melted vortex structures, will be investigated. For disordered networks, the effects of pinning in producing metastable vortex structures leading to glassy behavior will be explored.

To date, simulations have been carried out for two dimensional regular Josephson junction arrays with various values of applied magnetic field. I-V characteristics and resistivity were computed and related to vortex structure. Preliminary work on the behavior of flux line lattices in three dimensional networks has begun.

This research will greatly enhance our fundamental understanding of pinning and flux flow resistance in superconducting materials. The results will have impact in understanding the magnetic properties of the new high $T_c$ superconductors, and in the design of Josephson junction arrays for use as microwave detectors/generators.

Keywords: Flux Flow, Pinning, Vortex Motion, Superconductors

219. Energy Changes in Transforming Solids

FY 1990
$161,000

DOE Contact: Oscar P. Manley, (301) 353-5822
Stanford University Contacts: George Herrmann, David M. Barnett, (415) 723-4143

The objective of this research is to investigate problems of stressed deformable solids in which computations of energy changes and associated thermodynamic (or configurational) forces have important implications.

During the past year we have developed a computational routine capable of computing the energies of, and forces on dislocations in layered anisotropic media, which are important configurations of interest in modern integrated circuit technology. The theory of interfacial (Stoneley) waves in bonded piezoelectric half-spaces has been fully developed, as has also the theory and computations of so-called zero curative extraordinary transonic states in anisotropic elastic media. Orientations and elastic constant restriction admitting Type 3 transonic states have been delineated for five of the eight anisotropic crystal classes. Color computer graphics is now being used to produce three-dimensional views of slowness surfaces in anisotropic elastic and piezoelectric solids; this work has also led to the production of faster algorithms for determining the limiting speed which defines the first transonic state. In the coming year we intend to improve these graphics capabilities to include rotations and slicing, and to extend our elastic studies to deduce the behavior of interfacial crack tip singularities in anisotropic elastic and piezoelectric media.

Problems of composite materials consisting of single inclusions or two inclusions have been solved using a "circle theorem" developed previously and a "two-circle theorem" discovered in the past year. The latter theorem is now being used to study inclusions with either bonded or "slipping" interfaces. Using Noether's theorem, conservation laws based on non-classical transformations are being examined for their application to fracture and defect mechanics. Finally, our previous work on isothermal thermodynamics of stressed solids as applied to theories of damage in brittle solids is being extended to non-isothermal conditions.

Keywords: Stress Analysis, Materials Science

220. Nondestructive Testing

FY 1990
$252,549

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

The object of this research is to determine the usefulness of new optical methods, including photoacoustic and photothermal measurements as novel techniques in solid state research, notably for high critical temperature superconductivity.

The proposed research deals with the development of nondestructive techniques for characterizing the new high temperature superconducting materials. Those materials are difficult to characterize because they are polycrystalline, brittle, highly anisotropic, and inhomogeneous. The noncontracting photoacoustic and photothermal techniques developed in the preceding phase of this project can provide important information on the nature of the microstructure and grain boundaries which influence the superconducting properties.

Keywords: Nondestructive Evaluation, Acoustic Sensors

221. Effective Elastic Properties of Cracked Solids FY 1990
$53,978

DOE Contact: Oscar P. Manley, (301) 353-5822
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The knowledge of effective elastic properties of solids with cracks appears to be of increasing engineering importance. Extensive microcracking in structural elements working under conditions of high temperatures or irradiation, or microcracking in composite materials under fatigue conditions may noticeably reduce the stiffness of the material and make it anisotropic. Understanding and prediction of these changes are essential for proper design and strength and lifetime assessments. A new approach to many crack problems based on interrelating the average fractions of individual cracks is introduced. Its advantages are that it yields simple analytical results which are quite accurate up to very high crack densities and that it can be applied to crack arrays of arbitrary geometry. Relation between deterioration of elastic properties and "damage" is discussed.

Keywords: Fracture, Elasticity

222. Laser Diagnostics of Plasma Assisted Chemical Vapor Deposition (PACVD) Processes FY 1990
$175,217

DOE Contact: Oscar P. Manley, (301) 353-5822
United Technologies Research Center Contact: W. C. Roman, (203) 727-7590

The objectives of this research are to perform a comprehensive experimental investigation of the fundamental nonequilibrium reactive plasma assisted chemical vapor deposition (PACVD) process applicable to hard face coatings. Based on its superior erosion resistance, $TiB_2$ was selected as the initial coating for deposition onto a titanium alloy substrate (Ti-6Al-4V). In task I, novel non-intrusive laser diagnostic techniques (e.g., Laser Induced Fluorescence Spectroscopy (LIFS), and Coherent Anti-Stokes Raman Spectroscopy (CARS)) are being used to determine, *in situ*, the reactive plasma composition, temperature, and species concentration and distribution in the gas phase. Coupled with these experiments will be modeling of the plasma chemistry process. The second task includes use of Auger Electron Spectroscopy (AES), Ion Scattering Spectroscopy (ISS), Secondary Ion Mass Spectroscopy (SIMS) and other complementary techniques for detailed coating characterization. These are being combined with physical measurements of coating surface smoothness, hardness (state-of-the-art nanoindenter apparatus) and adherence (UTRC custom built pin-on-disc apparatus). These combined tasks will allow a correlation of the PACVD parameters with their required coating properties, thus providing a predictive capability that is severely lacking in the present science base of advanced protective coatings. Results to date include: (1) fabrication of a 5 kW rf PACVD reactor system integrated with a completely oil-free, high vacuum system; (2) exploratory spectral emission surveys for major molecular band and atomic line identification;

(3) development of a collinear, scanned, narrowband CARS system; (4) implementation of an ultramicrohardness tester and adhesion test apparatus; (5) initial characterization of $TiB_2$ and diamond coatings; and (6) first time CARS measurement of several key species (e.g., $B_2H_6$).

Keywords: Coating, Plasma Diagnostics

223. Thermodynamics of High Temperature Brines

FY 1990
$98,600

DOE Contact: William C. Luth, (301) 353-5822
Lawrence Berkeley Laboratory Contact: K. S. Pitzer, (415) 642-3472

This project covers theoretical and experimental studies concerning the thermodynamic properties of aqueous electrolytes at high temperatures. The components important in natural waters and brines are emphasized. The resulting data are important in understanding certain geothermal and other natural resources and in fission-product waste disposal. Moreover, this information has a wide range of applicability, since similar solutions arise in many industrial processes and in high-pressure steam power plants.

The experimental program involves measuring the heat capacities and heats of mixing or dilution of solutions exceeding 300 °C and pressures to 1 kbar. The database for the principal components of natural waters has now become adequate for the prediction of mineral solubilities in brines up to about 300 °C. Such calculations, based on the activity and osmotic coefficient equations of this project, were made for a number of systems containing Na+, K+, $Mg^{2+}$, $Ca^{2+}$, Cl-, OH-, $SO_4^{2-}$, and $H_2O$. Once the parameters are established for binary and common-ion ternary systems, no further parameters are needed for more complex brines, and calculations are truly predictive.

A theoretically based equation has been developed for the near-critical and supercritical properties of NaCl-$H_2O$. Parameters were fitted to the vapor-liquid coexistence surface for temperatures of 600 °C and compositions from pure $H_2O$ to that of the liquid on the three-phase line. Heat capacities and enthalpies were then predicted by this equation and agree satisfactory with the available experimental data.

Keywords: Electrolytes, Critical, Supercritical

224. Studies of the Interactions Between Mineral Surfaces and Ions in Solution

FY 1990
$88,740

DOE Contact: William C. Luth, (301) 353-5822
Lawrence Berkeley Laboratory Contact: D. L. Perry, (415) 486-4819

The X-ray fluorescence microprobe technique, using a synchrotron radiation source, has been employed to study the surface of oxidized galena (PbS) and its reactions with high oxidation metal ions in solution. These reactions, conducted at 100 °C in order to increase the kinetics and the extent of the reactions, are shown to vary greatly from the analogous reactions in which the reacting substrate is an unoxidized, "clean," galena surface. The resulting surfaces are observed to be much more heterogeneous than the comparable reactions involving the clean surfaces.

One good example of a reaction system that gives dramatic results in this series of studies is that of the solution interaction of aqueous chromium with the oxidized surface. Mapping of that reaction surface using the X-ray fluorescence microprobe indicates enriched chromium in areas that have been shown previously to include both hydrated chromium (III) oxide hydrates and mixed chromium-lead oxides. Past studies in this laboratory also indicated the existence of segregated islands on the surface that are enriched in chromium; the amount of chromium varies from as little as 35 pg/g to as much as 100 pg/g. Some of the chromium-rich islands at the highest concentrations are as wide as ~100 microns. Again, these variations merely mirror the difference in the chromium (III, VI) chemical phases on the galena surface.

It is clear from these experimental data that the galena surface involved in solution interface reactions as described here cannot be satisfactorily described as a homogeneous surface available for dissolution or other subsequent reactions. Rather, the solid/solution interface reaction processes involving these surfaces can only be modeled as ones which must includes a multiplicity of chromium (III), chromium (VI), and lead (II) phases. These (and related) reaction systems of metal ions will be studied further with respect to the reaction products, mechanisms, and kinetics. The synchrotron-related experimental work is being balanced with traditional X-ray photoelectron, Auger, and other types of spectroscopy in order to provide rigorous experimental data for input to such models.

Keywords: Chemisorption, Fluorescence, Synchrotron Radiation

225. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions

FY 1990
$147,900

DOE Contact: William C. Luth, (301) 353-5822
Lawrence Livermore National Laboratory Contact: D. G. Miller, (415) 422-8074

Transport of dissolved species in water by diffusion is of major importance to a wide variety of geochemical phenomena, including isolation of radioactive and chemical wastes, digenesis and ore formation, crystal growth, and dissolution kinetics for certain types of minerals. Activity coefficients are required for all chemical equilibrium calculations involving aqueous electrolyte solutions, including calculation of thermodynamic solubility products, calculation of Gibbs energies of formation for solid phases, calculation of vapor pressures of water above aqueous solutions, and speciation calculations. We have been making a variety of experimental measurements to provide some of the required data for aqueous binary and ternary electrolyte solutions at 25 °C: (1) Diffusion coefficients have been measured for the major and minor brine salts (except for $K_2SO_4$ and alkali metal carbonates) and mixtures of NaCl with $MgCl_2$ and with $SrCl_2$. (2) Osmotic coefficients have been measured for all of these electrolytes and for other binary and ternary systems, at least to saturation and generally to considerable supersaturation. (3) Solubilities were measured for many of the binary solutions using the isopiestic method. (4) Densities were measured for solutions used in the diffusion experiments.

This year our experimental program emphasized isopiestic measurements for aqueous mixtures of $NaHSO_4$ + $H_2SO_4$ and supplemented our earlier work for $NaHSO_4$ and $NAHSO_4$ + $Na_2SO_4$. Data now extend to about 15 mol $\cdot kg^{-1}$, which is considerably above the solubility limits, and should be completed this year. Previous results are restricted to 3.5 mol $\cdot kg^{-1}$ and lower, and were inadequate to characterize this complex system.

This year we completed the extraction of the diffusion data from all our experimental runs on aqueous NaCl-$MgCl_2$. These data are part of a 10-laboratory international collaboration on the transport properties of this system. Three experimental papers have been published, and one is in press. We have done an extensive analysis of mixture rules for conductance using NaCl-$MgCl_2$ data from the Argentine collaborators. We have examined deviations from "ideal" mixing rules for different conductance representations, including specific, molar, equivalent, and ionic strength conductances at either constant molarity, constant equivalent concentration, or constant ionic strength. The relationships between these three representations have been systematized. Deviations from the ideal mixture rules and the Van Rysselberghe-Nutting rule are smallest at constant normality.

Keywords: Electrolytes, Diffusion

226. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures

FY 1990
$108,460

DOE Contact: William C. Luth, (301) 353-5822
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Knowledge of the thermodynamic properties of electrolyte solutions at high temperatures is important in studies of geothermal systems, hydrothermal alteration processes, and element transport in deep brines such as those that have been encountered in the Continental Scientific Drilling Program (CSDP). Properties to at least 473 K for carbonates, hydroxy species, and organic complexes are especially needed to model cementation, mineral digenesis, and element transport in sedimentary basin evolution. The purpose of this investigation is to determine the activity coefficients of geochemically important ionic species in aqueous solutions over a wide range of composition and temperature.

An automated, flow calorimeter has been constructed to measure the heat capacities of concentrated, electrolyte solutions to 673 K and 40 MPa. Heat capacity data can be integrated to yield enthalpy and total free energy information by using literature data available at room temperature to evaluate the integration constants. The total free energies can be used directly in calculations of mineral/solution equilibria. If the data can be extrapolated to infinite dilution (this is proving to be a serious problem for electrolytes other than the 1-1 charge type at temperatures above 500 K), calculation of standard state properties and activity coefficients is possible. These can then be treated using Pitzer's equations to provide a compact model for mixed electrolyte solutions at high temperatures.

Heat capacity data have been obtained for the systems $NaCl$-$Na_2SO_4$-$H_2O$, $NaOH$-$H_2O$, and $Na_2CO_3$-$NaHCO_3$-$NaCl$-$H_2O$ to 40 MPa and 598 K and sodium acetate to 40 MPa and 473K. Heat capacities for NaOH have been combined with high quality enthalpy of dilution measurements by J. M. Simonson (ORNL) to provide standard state values. These are also of interest because they can be used to fix the standard state values for HCl(aq) through the reaction to form NaCl and $H_2O$. Heat capacities for $NaHCO_3$-$Na_2CO_3$-$Na_2CO_3$-$H_2O$ are presently being combined with enthalpy data from ORNL to provide a complete thermodynamic model for this system.

Keywords: Electrolytes, Heat Capacity

227. Solubilities of Calcite and Dolomite in Hydrothermal Solutions FY 1990 $98,600

DOE Contact: William C. Luth, (301) 353-5822
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Highly accurate measurements of the solubilities of calcite and dolomite are needed in order to model digenesis and the development of secondary porosity in sedimentary basins, because calcite is a common digenetic phase and the dolomitization of limestone involves a 14.2 percent volume reduction. Calcite is also one of the major scales which develop in geothermal reservoirs and production wells. Previous studies demonstrated that the logarithm of the equilibrium constant for the reaction $CaCo_3 + CO_2 + H_2O \rightleftharpoons Ca^{2+} + 2HCO_3^-$ at 300 bars total pressure decreases from -4.86 at 100 °C to -9.98 at 300 °C. At 1000 bars, the equivalent log K values are 3.98 at 100 °C and -8.05 at 300 °C. For the reaction $1/2CaMg(CO_3)_2 + CO_2 + H_2 \rightleftharpoons 1/2Ca^{2+} + 1/2Mg^{2+} + 2HCO_3$, the log values at 300 bars range from -4.35 at 100 °C to -8.56 at 300 °C. This year, these reactions were studied at 50 °C and 300 bars, giving log K values of -4.09+0.02 for the calcite reaction and -.41+0.02 for the dolomite reaction. The kinetics of dissolution are extremely sluggish at these conditions, resulting in very time-consuming experiments. A series of Ca-Mg cation exchange experiments with calcite-dolomite mixtures at 25, 50, and 70 °C and 1 bar were also initiated during this period. A value of 0.445 was obtained for the equilibrium log $(Ca^{2+}/Mg^{2+})$ value at 50 °C. Accurate data of this type are needed in order to predict the onset of dolomitization or dedolomitization in coupled reaction-transport computer codes.

Keywords: Carbonates, Solubility

228. Salinity Effects on Oxygen and Hydrogen Isotope Partitioning Between Geothermal Brines and Other Phases at Elevated Temperatures FY 1990 $63,104

DOE Contact: William C. Luth, (301) 353-5822
Oak Ridge National Laboratory Contact: D. J. Wesolowski, (615) 574-6903

Equilibrium isotopic fraction factors for D/H and $^{18}O/^{16}O$ exchange between silicate minerals and NaCl solutions have been estimated to 300 °C, based on sparse literature data and our results for liquid/vapor D/H exchange as a function of NaCl concentration at 70 and 100 °C. Between 25 ° and 300 °C, salinity effects for both oxygen and hydrogen exhibit a complex, nonlinear temperature-composition dependence that is difficult to predict from electrolyte theory. The salt effect can be as large as 3.5 permil for oxygen and 12 permil for hydrogen at temperatures above 150 °C. If ignored, the salt effect associated with a 4 molal NaCl solution can lead to errors in geothermometry estimates of 30 ° to 50 °C. In boiling hydrothermal fluids, the presence of NaCl profoundly influences the $^{18}O/^{16}O$ and D/H partitioning between liquid and vapor. As an extreme, at 250 °C in the pure water system, the $\delta^{18}O$ values of liquid and vapor continually increase as boiling proceeds, whereas with NaCl present the general trend is one of depletion in $\delta^{18}O$ for both liquid and vapor. Quartz precipitated from these two systems would mimic these dissimilar trends. The magnitude of the salinity effects on rates of exchange and equilibrium fractionations are far too great to be ignored and must be accounted for when modeling data from natural systems and experiments.

A major effort was expanded during this period in assembling and critically reviewing the available data, including past results from this program, on the effect of dissolved NaCl on the rates of D/H and $^{18}O/^{16}O$ exchange and the equilibrium fractionations between aqueous NaCl solutions and other phases, including silicate minerals and the vapor phase. We have demonstrated that rates of isotopic exchange are greatly enhanced by interaction of a mineral or rock with NaCl solutions relative to interaction with pure water. This rate increase is due to either the more rapid transformation of the reactant phase to a new phase (e.g., sanidine to albite) or recrystallization of the reactant compared to pure water systems. For example, at 250 °C the rate of oxygen isotopic exchange for sanidine-$H_2O$ is $10^{-9.0}$ moles O/m $^2$/sec versus $10^{-7.8}$ for the interaction of sanidine with 2-3 molal NaCl solutions. The time required to obtain 90 percent equilibration in the systems anidine-$H_2O$-NaCl, quartz-$H_2O$-NaF, and calcite-$H_2O$-$NH_4Cl$ has been calculated using a modified surface-exchange rate model for closed systems. These calculations indicate that below 300 °C the rate of isotopic equilibration can be 2 to 50 times faster than in pure $H_2O$, depending on the mineral and type and concentration of electrolyte.

Keywords: Brines, Isotopic Composition

229. Advective-Diffusive/Dispersive Transport of Chemically Reacting Species in Hydrothermal Systems

FY 1990
$120,000

DOE Contact: William C. Luth, (301) 353-5822
University of California at Berkeley Contact: H. C. Helgeson, (415) 642-1251

Understanding the chemistry of fluid flow and water-rock interaction in geochemical processes requires thermodynamic and transport properties of hydrothermal fluids, as well as comprehensive mass transfer computer codes. Toward this end we have focused during the past year on characterizing speciation in concentrated supercritical aqueous electrolyte solutions, generating tracer diffusion coefficients for organic species and developing computer algorithms to calculate the growth rate of hydrothermal alteration zones.

Revised interpretation of conductance measurements reported in the literature indicates that the solute in supercritical aqueous alkali metal halide solutions is present predominately as single ions and neutral ion pairs only in the dilute concentration range at supercritical pressures and temperatures. For example, calculations indicate that the degree of neutral ion pair formation in NaCl solutions at 600 °C and 2 kbar maximizes with increasing concentration at ~.02 M and becomes negligible at higher concentrations (1 M), where triple ions predominate. This behavior is a consequence of the low dielectric constant of $H_2O$ at supercritical temperatures and pressures. By analogy with the behavior of electrolytes in low-dielectric constant solvents at low temperatures and pressures, it appears likely that in addition to triple ions, higher order complexes such as quadruple, quintuple, etc. species sequentially predominate with increasing concentration in supercritical solutions of single electrolytes.

Analysis of tracer diffusion coefficients ($D^\circ$) for aqueous organic species reported in the literature indicates that $D^\circ$ can be described as a linear function of the reciprocal square root of the alkyl chain length of the species. The temperature dependence of $D^\circ$ can be represented by a modified Arrhenius equation. These two relations permit calculation of tracer diffusion coefficients for a wide variety of aqueous organic species at temperatures to 350 °C.

The growth of hydrothermal alteration zones can be characterized as a function of time and distance using a numerical algorithm which permits simultaneous solution of homogeneous equilibrium constraints and diffusion equations coupled to reversible and irreversible mineral dissolution/precipitation reactions. A computer code is being developed to compute the diffusional growth rate of hydrothermal alteration zones using a quasi-stationary state approach to integrate the mass transport equations over geologic time frames. The rate at which the primary rock reacts is limited in the code by kinetic rate laws for the hydrolysis of minerals. The algorithm will be used to study alteration halos such as those associated with hydrothermal veins in porphyry copper deposits and metamorphosed dolomites.

Keywords: Electrolytes, Petroleum, Dissociation

230. Rock Mechanics: Thermal Stress Microfracturing of Crystalline and Sedimentary Rocks

FY 1990
$108,460

DOE Contact: William C. Luth, (301) 353-5822
LLNL Contact: B. P. Bonner, (415) 422-7080

Acoustic emissions (AE) are used in the analysis of microcrack generation in brittle materials. Microfracturing occurs due to internal thermal stress arising from local mismatches in elastic constants and thermal expansion. AE studies are accompanied by measurements of frequency dependent ultrasonic velocity.

Keywords: Brittle Materials, Microfracturing, Acoustic Emission, Thermal Stress

231. Diffusion in Silicate Materials

FY 1990
$88,740

DOE Contact: William C. Luth, (301) 353-5822
LLNL Contact: F. J. Ryerson, (415) 422-6170

Determination of diffusion profiles (Pb, Sr, Nd) in silicate minerals at 600C<T<900C through ion implantation. Ion implantation results in radiation damage with dramatically increased diffusion coefficients with activation energies comparable to published (non ion-implantation) values.

Keywords: Diffusion, Silicate, Activation Energy

232. Rheology of Melts

FY 1990
$167,620

DOE Contact: William C. Luth, (301) 353-5822
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University of Minnesota Contact: D. A. Yuen, (612) 624-1868

Rheometric experiments using a concentric cylinder rheometer on silicate melts and crystal-liquid mixtures, with and without dilute concentrations of air bubbles. Research is directed toward understanding recent caldera-type volcanic eruptions, and involves modeling using a large-amplitude Lagrangian formulation. Model assumes elastic-visco-plastic rheology and includes thermal equations governing heat transport and mechanical dissipation.

Keywords: Rheology, Magma, Silicate, Liquid

233. Microcrack Growth in Crystalline Rock

FY 1990
$69,020

DOE Contact: William C. Luth, (301) 353-5822
Lawrence Berkeley Laboratory Contact: L. R. Myer, (415) 486-6456

Mechanism of microcrack growth in brittle rock under compressive stress. Experimental study aimed at obtaining quantitative data under triaxial compression. Assessment of role of pore collapse and compaction.

Keywords: Microcracks, Microfractures, Brittle Material

234. Experimental Database and Predictive Theories for Thermodynamic Properties of Aqueous Solutions

FY 1990
$55,943

DOE Contact: William C. Luth, (301) 353-5822
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Measurements of the apparent molar heat capacity of aqueous solutions of $H_2S$, $CO_2$, and $CH_4$ are being made at twelve temperatures from 25 ° to 450 °C and at pressure near 350 bar. Measurements of the apparent molar volume of aqueous solutions of $H_2S$, $CO_2$, and $CH_4$, are being made at the same twelve temperatures and at two different pressures. These measurements will accurately define the equilibrium properties of aqueous solutions of these gases at temperatures up to 450 °C and pressures to 350 bar. These solutes are crucial reactants in a wide variety of geochemical processes and an accurate knowledge of their thermodynamic properties will permit a much better understanding of the driving forces for these processes. The measurements will double the amount of information available on volumes and heat capacities of aqueous nonelectrolytes at high temperatures. Theoretical models capable of representing these data and extrapolating them to higher temperatures and pressures are being investigated. Correlations and theoretical models that will allow the estimation of the properties of other nonelectrolytes of geochemical interest are also being investigated.

Keywords: Aqueous Solutions, Heat Capacity

235. Physical Characterization of Magma Samples

FY 1990
$ 0

DOE Contact: William C. Luth, (301) 353-5822
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The main objectives of this project are: 1) to employ ultrasonic interferometry techniques to measure velocity and attenuation in natural and synthetic silicate melts; 2) to investigate interrelationships between the various physical, elastic and anelastic, and thermodynamic properties of silicate melts; and 3) to develop a Brillouin scattering technique for measuring the elastic and anelastic properties of melts in a wide range of temperature and pressure.

To accomplish these goals, laboratory studies are being conducted on natural rocks and synthetic silicate samples and their melts in three research areas: 1) characterization of physical, elastic and anelastic ($V_p$, $V_s$, $Q^{-1}$), and electrical properties of samples from Kilauea Iki lava lake and other related types of basalts; 2) development of Brillouin and Raman scattering measurements on synthetic and natural silicates and their melts, first as a function of temperature and then as a function of temperature and pressure, in an effort to understand the structure-property relationships in silicate melts; and 3) investigation of electrical conductivity of molten and partially molten rocks and silicates to understand the role of partial melting.

Ultrasonic measurements have been carried out on the melts of several types of natural rocks (basalts and komatiites) and on selected synthetic samples in the systems diopside ($CaMaSi_2O_6$)-anorthite ($CaAlSi_2O_8$) and albite ($NaAlSi_3O_8$)-anorthite ($CaAlSi_2O_8$) anorthite ($CaAlSi_2O_8$)-diopside ($CaMgSi_2O_6$) and to ~1600°C and in the frequency range 3-22 MHz. These measurements have enabled us to establish the velocity-density-composition (Birch's linear law) and attenuation-temperature-frequency systematics and to interpret the viscoelastic properties (viscosity, relaxation time, etc.) in terms of their composition and structure. We are now turning to employing the recently set up Brillouin scattering system and diamond anvil to study the compressibility of silicate melts at high pressures. The ultrasonic and Brillouin scattering results, to be extended to high pressures in the future, will provide important thermodynamic parameters (e.g., compressibility) for these melts at high pressure. The electrical conductivity measurements on the Kilauea Iki basalts have now been completed. In progress are the measurements on the nepheline-sodium disilicate ($NaAlSiO_4$-$Na_2SiO_3$) system to ~1000°C to determine the effect of partial melting (solidus = 768°C) on the electrical properties.

Keywords: Silicates, Ultrasonics

236. Investigations of Ultrasonic Surface Wave Interaction with Porous Saturated Rocks

FY 1990
$54,000

DOE Contact: William C. Luth, (301) 353-5822
Ohio State University Contact: L. Adler, (614) 292-1974

In this research project we conducted an investigation of surface waves and bulk waves with fluid-filled porous materials. First, we concentrated on the propagation of various surface waves on fluid-saturated porous materials, both synthetic and natural rocks. We developed two novel techniques for surface wave studies. One of the techniques was based on the mode conversion of bulk waves on corrugated surfaces, which the second one used direct excitation of surface waves. In order to extend our surface wave studies to other guided wave modes, we formulated the general problem of reflection and transmission of elastic waves through various interfaces of fluid-filled porous materials. We carried out numerical calculations and verified, by experiment, the angular behavior of the reflection and transmission coefficients for both fast and slow waves, as well as for shear waves. We have shown that although the boundary conditions (i.e., open or closed pores at the interface) affect the strength of the transmitted slow waves through the porous materials, a more major role is played by volumetric attenuation. To increase the detectability of slow waves we introduced another new method based on the generation and detection of leaky Lamb waves. We have shown, both experimentally and theoretically, that the lowest Lamb mode is due to the slow wave compared to the more conventional bulk technique. We developed a new technique based on the transmission of airborne ultrasonic waves through air-saturated porous plates in order to observe slow waves in natural rocks. To the best of our knowledge, our preliminary results represent the first irrefutable evidence of slow waves in fluid-saturated natural rocks, such as different types of sandstones.

Keywords: Ultrasonics, Lamb Waves

237. Zircons and Fluids: An Experimental Investigation with Applications for Radioactive Waste Storage

FY 1990
$59,811

DOE Contact: William C. Luth, (301) 353-5822
Virginia Polytechnic Institute and State University Contact: A. K. Sinha, (703) 231-5580

During the second year of our project we have completed the physical and chemical characterization of synthetic zircons, as well as 40 natural zircons of varying ages (2700 m.y. to 300 m.y.). Two zircon samples with very distinct total alpha dosages have been investigated for uranium and lead isotopic stabilities at pressures up to 6 kbar and 600 °C. Although the composition of fluids plays a marked role in the removal of uranium and lead from the zircons, there is a predictable relationship between the amount of uranium removed from the zircon and the total alpha dosage. For a given experimental solution (2M NaCl) the strongly metamictized zircons (D° = $1.5 \times 10^{15}$, uranium = 2000 ppm) lost over 50 percent uranium, while another test sample with lower uranium content (215 ppm) lost approximately 30 percent. Out results support our working model that stability of $ZrSiO_4$ in a fluid medium is strongly correlated to total alpha dosage and must be a major factor in designing chemical forms for waste repository hosts.

We have also completed preliminary studies of the solubility of crystalline zircons at low pressures (25 bars) and temperatures (200 °C). This environment more closely approximates waste repository conditions. Our solubility data suggest a first order dissolution rate low. The constant ratio in molar Si/Sr (above unity) seen in our experiments suggests that $ZrOCl_2$ may not be as soluble in 3N NCl as in HCl solutions below normality of one.

From these studies we are developing a comprehensive model of the stability of zircons at varying P-T-X conditions.

Keywords: Zircons, Uranium, Hydrothermally Induced Mobility

238. PVTX Properties of Fluid Systems: $NaCl-CaCl_2-H_2O$ FY 1990
$78,000

DOE Contact: William C. Luth, (301) 353-5822
Virginia Polytechnic Institute and State University Contact: R. J. Bodnar, (703) 961-7455

Experimental data on the PVTX properties of fluids provide the basic information required to develop quantitative models to describe the physical and thermodynamic behavior of natural fluids. These models in turn facilitate the understanding of water-rock and fluid-magma interactions that occur in the Earth's crust.

The system $NaCl-CaCl_2-H_2O$ provides a reasonable approximation of fluids in sedimentary basins (oil-field brines) and many higher temperature metamorphic and magmatic environments. We have begun a study of this important system as part of our continuing program to determine the PVTX properties of geologically applicable fluid systems over the range of pressure and temperature conditions encountered in crustal environments. Experiments have been conducted to determine phase relations in the ice-stable region of this system under vapor-saturated conditions, and an equation has been developed to describe ice-liquid equilibrium (liquidus) as a function of temperature. Densities of $NaCl-CaCl_2H_2O$ solutions have been determined as 298 and 308 K and 0.1 MPa for ionic strengths ranging from 0.1 to 19.2 mol $\cdot kg^{-1}$, and along the 7 and 40 MPa isobars from 298 to 523 K using a vibrating U-tube densimeter apparatus in the Chemistry Division at Oak Ridge National Laboratory. Experiments to determine the positions of isochores at elevated temperatures and pressures using the synthetic fluid inclusion technique are in progress. These data will be combined with PVTX data obtained using the U-tube technique at lower pressures and temperatures to develop an equation of state for the system $NaCl-CaCl_2H_2O$.

Results available to date suggest that previously published data for PTX relations in the ice-stable region may contain significant errors. Interpretation of fluid inclusion compositions from the Salton Sea Geothermal System (SSGS) using the older data indicates significant differences between present-day fluids and those present at some time in the past when the inclusions were trapped. The discrepancy is eliminated if the fluid inclusion measurements are reinterpreted using ice-liquidus data from this study. Whether or not the geothermal fluids have changed with time has important implications for the evolution of the SSGS and for hydrologic models used to describe fluid flow characteristics of the SSGS.

Keywords: Geological Fluids, Thermodynamic Properties

Materials Structure and Composition

239. Silicate Thermochemistry

FY 1990
$123,000

DOE Contact: William C. Luth, (301) 353-5822
Princeton University Contact: A. Navrotsky, (609) 452-4674

The purpose of this work is to expand our data base and understanding the thermochemistry of minerals and related materials through a program of high temperature reaction calorimetric studies. This year a good deal of effort has been put into expanding and developing new calorimetric techniques which will enable us to integrate data on low temperature hydrous phases and on high temperature anhydrous minerals, glasses, and melts. The dissolution of water-bearing and carbonate-bearing phases in molten lead borate is being characterized in detail. Solution calorimetry by R. Rapp of alkali and alkaline earth carbonates provides a reference state for heats of solution involving the alkali and alkaline earth oxides and paves the way for studies of carbonate thermochemistry. Overcoming kinetic problems in the dissolution of rare earth oxides and titanium and zirconium dioxides enables us to determine heats of formation of minerals containing these elements, work on zircon is in progress (A. Ellison).

Several projects involving hydrous phases have been completed. In addition to the tremolite-richterite join studied by A. Pawley last year, S. Circone has completed X-ray, NMR, thermogravimetric, spectroscopic, and solution calorimetric studies of the Mg-Tschemak substitution along the Mg-Al-phlogopite join. $KMg_3AlSi_3O_{10}(OH)_2$ - $KMg_2AL_3Si_2O_{10}(OH)_2$, using synthetic samples. W. Carey performed a calorimetric study of the energetics of water in cordierite, and P. Maniar studied a series of silica gels and some synthetic pure silica zeolites. These studies taken together begin to unravel the simultaneous energetic effects of coupled ionic substitutions, of framework topology, and of water content in complex chain, sheet, and frame silicates. The thermodynamic properties of such phases are important in digenesis, metamorphism, rock-water interactions, and nuclear waste disposal.

A. Ellison's work on glasses has focused on the system $K_2O$-$La_2O_3$-$SiO_2$. Several joins in this system show virtually linear heats of solution, implying nearly zero heats of mixing. Coupled with Raman spectra, the EXAFS studies, and with the energetics of phase separation, these observations suggest a constant local environment for La and substantial local "phase ordering" such that macroscopic immiscibility represents a change in the size of domains already present rather than major structural rearrangement. Calorimetric data for these and other simple three-component glasses have been used to predict the structural features and heats of mixing in nuclear waste glasses, and to suggest that heats of mixing between these commercial multicomponent glasses are generally small.

To better understand possible coordination geometries in glasses and crystals containing two or more different cations, A. Ellison has been developing computerized enumeration schemes based on generalizations of Pauling's rules.

Keywords: Silicates, Glasses, Thermodynamics

Division of Advanced Energy Projects

Materials Preparation, Synthesis, Deposition, Growth or Forming

240. Gas Jet Deposition of Metallic, Semiconducting and Insulating Films — FY 1990 $150,000

DOE Contact: Walter M. Polansky, (301) 353-5995
Schmitt Technology Associates Contact: Bret Halpern, (203) 432-4376

Gas Jet Deposition (GJD) is a new method for depositing thin films at high rate and controlled energy. The basic physics of GJD will be investigated in order to develop its technological capabilities. GJD deposits films by "seeding" atoms or molecules into a free jet expansion, e.g., of helium, and directing the jet at a substrate at relatively high pressure. GJD promises many advantages over established methods. Deposition rates of 10 microns per minute have been attained, and microns per second should be within range. The impact energy of depositing species can be gas dynamically controlled over a range of electron volts, so that film properties can be influenced during deposition. The substrate, which can be almost any material, can remain cool during deposition. Film composition and doping profile can be easily varied. Clusters can be deposited as well as atoms and molecules. GJD is flexible, and any metal, semiconductor, or insulator that can be seeded in the free jet can be deposited. The combination of these features in one method makes GJD singularly versatile. The goal of this project is to explore the feasibility of GJD as the basis of a usable technology. To do this, the fundamentals of GJD will be investigated. In particular, its high rate and impact energy control and the GJD apparatus will be refined. The properties of the films produced will be determined.

Keywords: Coatings and Films, Gas Jet Deposition

241. Growth of High $T_c$ Superconducting Fibers Using a Miniaturized Laser-Heated Float Zone Process — FY 1990 $375,000

DOE Contact: Walter M. Polansky, (301) 353-5995
Stanford University Contact: Robert S. Feigelson, (415) 723-4007

The primary objective of this project is to thoroughly explore the potential of the laser-heated pedestal (float zone) growth method for the preparation of flexible wires (fibers) of the new copper-oxide ceramic superconductors, in particular the Bi containing compounds which are capable of carrying high currents at temperatures above 77 °K. This method, which involves drawing wires directly from a melt, has many advantages over other methods, most important of which is that it allows precise control of the growth process through the control of melt composition. Critical issues which will be considered in this superconducting fiber program include (1) determining the most suitable compositions to be grown, (2) the maximum allowable growth velocity which can be used to grow fibers with high $T_c$, and (3) the maximum length of fiber which can be produced. To address these issues, the program will involve an in-depth study of (1) the thermodynamic and kinetic factors which affect growth rate and the properties of the fibers produced, (2) the development of an advanced fiber growth system which will permit better control of system parameters, and (3) the development of techniques to enhance fiber throughput via increased growth velocity, postgrowth heat treatments, and the possibility of growing many fibers simultaneously.

Keywords: Superconductivity, Laser-Heated Pedestal Growth

Materials Properties, Behavior, Characterization or Testing

242. Production of Fuels and Chemicals From Methane — FY 1990 $247,000

DOE Contact: Walter M. Polansky, (301) 353-5995
Argonne National Laboratory Contact: Victor A. Maroni, (708) 972-4547

In this project research is being carried out to develop novel bifunctional catalysts (BFCs) that can convert methane to fuels (e.g., liquefied petroleum gas or gasoline) and large volume industrial chemicals. The goal is to produce a catalyst that operates efficiently under moderate conditions of temperature (<500 °C) and pressure (<10 atm), and for extended periods of time, without need for frequent regeneration or replacement. The BFC concept involves integrating into one material the properties of C-H bond activation and product-selective chemical synthesis. Several types of C-H bond activation catalysts that rely on unique oxidation state chemistries and coordination geometries are employed in combination with molecular sieve materials having well defined intracrystalline pores and channels that constrain the size and shape of the active catalytic species contained therein and the chemical species formed therein. This research is expected to culminate in a demonstration of the feasibility of efficient conversion of methane to a representative fuel and/or to one or more of the top 50 commodity chemicals.

Keywords: Catalysts, Molecular Sieves

Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program was established in compliance with the Small Business Innovation Development Act of 1982, Public Law 97-219. The program is designed for implementation in a three-phase process, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is about six months and awards are limited to $50,000. Phase II is the principal research or research and development effort, and awards can be as high as $500,000 for work to be performed in periods of up to two years. Under Phase III, commercial applications of the research or research and development are to be pursued by small businesses with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or processes desired by the Government.

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

The work supported in this program represents high-risk research, but the potential benefits are also high if the objectives are met. Brief descriptions of all DOE SBIR projects (not just those of interest in materials research) are given in the following publications: Abstracts of Phase I Awards, 1990 (DOE/ER-0472), Abstracts of Phase II Awards, 1990 (DOE/ER-0467), and Abstracts of Phase II Awards, 1989 (DOE/ER-0418). Copies of these publications may be obtained by calling Mrs. Gerry Washington on (301) 353-5867.

## OFFICE OF ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT

In November 1989 the Department consolidated into a new Office of Environmental Restoration and Waste Management (EM) waste management and waste treatment activities formerly managed by portions of the Office of Nuclear Energy and the Office of Defense Programs. These activities include waste treatment technology and specific project operations.

### Division of Waste Management Projects

The objective of the Division of Waste Management Projects is to conduct waste management activities for ending interim storage of high-level waste and achieving permanent disposal of high-level waste. Defense wastes were generated by atomic energy defense activities at three Departmental operating locations: the Savannah River Site in South Carolina, the Hanford Site in Washington, and the Idaho National Engineering Laboratory in Idaho. Additionally, Congress directed the Department in 1980 to demonstrate the solidification of liquid high-level waste at West Valley (New York) which originated at the nation's only commercial plant to reprocess spent nuclear fuel. At all four sites there are major programs in various stages of completion which will immobilize the high-level waste preparatory to geologic disposal. All four projects are managed by this Division.

At Savannah River and West Valley, high-level waste will be immobilized in a borosilicate glass prepared in a liquid-fed ceramic joule-heated melter. Hanford is planning to use the same waste form and process, but the project is in the conceptual design stage. At Idaho, the merits of several alternative waste management strategies are being evaluated. A strategy will be selected in compliance with the National Environmental Policy Act (NEPA) process for disposal of Idaho high-level waste.

The Defense Waste Processing Facility at Savannah River is beginning nonradioactive operations in preparation for radioactive operation in 1993. West Valley is constructing the vitrification cell. For these two projects, materials research focuses on incremental improvements in the waste form durability based on a reference formulation chosen some time ago. Hanford project is now studying pre-treatment options for most effectively preparing the several chemically-varied types of waste for partition between a high-activity stream which will be vitrified and a low-activity stream which will be immobilized in a grout or cement waste form.

Materials Preparation, Synthesis, Deposition, Growth or Forming

243. Technical Support to West Valley Demonstration Project FY 1990 $1,100,000

DOE Contact: T. W. McIntosh, (301) 353-7189
PNL Contact: W. A. Ross, (509) 376-3644

Pacific Northwest Laboratory (PNL) provides technical assistance to the West Valley demonstration project in characterizing high-level waste samples taken from the West Valley tanks; characterizing operating conditions for ion exchange processes that remove cesium and plutonium from the high-level liquid supernate; developing an empirical model which relates borosilicate glass composition to the chemical durability of the final waste form (including both preparation and testing of materials and the statistical analysis of the results to allow modeling); and characterizing individual process operations to show overall control of the vitrification process and the final waste form.

Keywords: Ion Exchange, Borosilicate Glass, Process Control, Radioactive Waste Host

Materials Properties, Behavior, Characterization or Testing

244. Materials Characterization Center Testing of West Valley Formulation Glass

FY 1990 $500,000

DOE Contact: T. W. McIntosh, (301) 353-7189
PNL Contact: S. C. Marschman, (509) 376-3569

Materials Characterization Center (MCC) is evaluating the chemical durability of glasses whose compositions are within the expected range of composition of the West Valley Demonstration Project borosilicate glass waste form. These include nonradioactive glass containing surrogate elements for the radionuclides and radioactive glass doped with appropriate radionuclides. The MCC also began testing of a small sample of glass containing actual West Valley high-level waste. MCC continues to provide assistance to West Valley relative to enhancing the quality of their analytical data.

Keywords: Radioactive Waste Host

245. Development of Test Methods and Testing of West Valley Reference Formulation Glass

FY 1990
$900,000

DOE Contact: W. S. Ketola, (716) 942-3414
CUA Contact: P. B. Macedo, (202) 635-5327

Vitreous State Laboratory of the Catholic University of America (CUA) continues to develop test methods for nonradioactive and radioactive borosilicate glass waste forms for the West Valley Demonstration Project and is studying means to maximize the region of acceptable quality around the point of optimal durability for the borosilicate glass waste form.

Keywords: Radioactive Waste Host

246. Process and Product Quality Optimization for the West Valley Waste Form

FY 1990
$250,000

DOE Contact: W. S. Ketola, (716) 942-4314
AU Contact: L. D. Pye, (607) 871-2432

Alfred University is studying properties and crystallization behavior of the West Valley borosilicate glass reference composition in anticipation of providing methods for control of product quality during routine manufacture of the West Valley Demonstration Project waste form

Keywords: Radioactive Waste Host

247. Waste Form Qualification

FY 1990
$6,000,000

DOE Contact: M. Dev, (509) 376-3412
WHC Contact: S. Schaus, (509) 376-8365

These studies provide fundamental data for start-up of the Defense Waste Process Facility, for waste compliance activities, and for acceptance of borosilicate glass at a repository. Site specific testing is included.

Keywords: Waste, Waste Form, Borosilicate Glass, Waste Acceptance Specifications

248. Immobilization, Volume Reduction, and In-place Stabilization FY 1990
$2,000,000

DOE Contact: M. Dev, (509) 376-3412
WHC Contact: S. Schaus, (509) 376-8365

These studies provide information about the process flowsheets for treatment of high-level waste at the Hanford Site and Idaho National Engineering Laboratory. The focus is on reduction of volume of immobilized waste. These studies include waste characterization, retrieval technology, and waste processing. Technology for in-place stabilization is being investigated where appropriate in order to ensure that disposal strategies include all technically feasible options.

Keywords: High-level Waste, Volume Reduction, In-Place Stabilization

# OFFICE OF NUCLEAR ENERGY

The Office of Nuclear Energy conducts materials research and development through 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 Uranium Enrichment

The specific statutory authority which established the Department of Energy's role in the enrichment of uranium is the Atomic Energy Act of 1954, as amended. The goal of the Uranium Enrichment Program is to maintain this activity as a strong viable enterprise retaining a market share that preserves a long term competitive position. It is intended that these services be done for worldwide commercial and United States defense customers in an economical, reliable, safe, secure, and environmentally acceptable manner that will ensure a reasonable return on the Government's investment.

Materials R&D activities within the Office of Uranium Enrichment are varied and, for the most part, classified Restricted Data. In FY 1990, approximately $20.5 million was used in these endeavors and about $25 million is planned for FY 1991. Paragraph summaries of these activities are presented in the second part of this report. The DOE contact is A. P. Litman, (301) 353-5777.

## Gaseous Diffusion

Uranium as found in nature contains about 0.7 percent uranium 235 and the remainder is essentially non-fissionable uranium 238. The fissionable characteristics of uranium 235 are necessary and useful for power reactor fuel. To date, most nuclear reactors designed for producing electrical power require uranium 235 concentrations between 2 and 5 percent. Presently, uranium is enriched to the desired uranium 235 assay levels in gaseous diffusion plants. These plants operate on the principle that lighter weight gaseous isotopes have slightly higher average velocities and thus can be made to diffuse through a porous barrier more rapidly than heavier species. Two streams can be created, one enriched in the lighter isotope and one depleted. Because enrichment for a single cycle, or stage, is very small, a cascade of stages is required. For example, a plant constructed for producing 4 percent assay U-235 would contain about 1200 stages. Although many other methods for enrichment are still being investigated and another production technique is being used in parts of Europe, diffusion plants today still provide approximately 90 percent of the world's enrichment services. 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

249. Gaseous Diffusion: Barrier Quality

FY 1990
$2,053,000

These studies include evaluation of the short- and long-term changes in the separative capability of the gaseous diffusion barrier and methods to recover and maintain barrier quality in the production plants. This activity is a long-term undertaking and will be maintained at appropriate levels of effort in the future.

Keywords: Nuclear Fuel Isotopic Separations, Gaseous Diffusion, Barrier, Uranium

250. Gaseous Diffusion: Materials and Chemistry Support

FY 1990
$3,060,000

This activity involves the routine materials and chemistry support for the diffusion plants. It includes the characterization of contaminant-process gas cascade reactions, the physical and chemical properties of $UF_6$ substances. Also, the work incorporates studies of the corrosion of materials, failure analyses, improving trapping technology, and alternative materials replacement.

Keywords: Nuclear Fuel Isotopic Separations, Uranium, Gaseous Diffusion

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

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

In June 1985, DOE selected U-AVLIS for further development and possible future deployment into the uranium enrichment enterprise. The primary emphasis for the U-AVLIS program in FY 1990 was to continue activities that will enable a demonstration of U-AVLIS in full size equipment in 1992. This demonstration will provide a base of technical and economic information adequate to accomplish three goals: (1) support a conceptual design for a U-AVLIS production plant, (2) establish a high confidence plan for integration of U-AVLIS into the nuclear fuel cycle, and, (3) allow a U-AVLIS production plant deployment decision. Available resources in FY 1990 were focused on these goals and the activities included operation of large test beds, key subsystems, and a full size separator. As shown below, the

U-AVLIS materials activities in FY 1990 were in support of the separator system and the uranium processing activities. The latter technologies will have strong economic leverage for a U-AVLIS production plant and are receiving more attention this year. The overall goal of uranium processing is to develop and demonstrate low-cost paths for integrating the U-AVLIS metal feed and product into the existing uranium oxide/fluoride nuclear fuel cycle.

251. U-AVLIS: Separator Materials | FY 1990 | $5,400,000

This activity includes the selection and testing of alternative candidate structural and component materials and coatings for the U-AVLIS separator system. It also supports the fabrication of full size separator components and subsystems for verification tests, plus the off line operation of a full size separator.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

252. U-AVLIS: Uranium Processing | FY 1990 | $10,000,000

This past year experiments and design studies concentrated on alternatives for preparation of U-AVLIS feed from uranium ore and the selection of a baseline feed preparation process. To support the back end of the fuel cycle, the design of a demonstration system for U-AVLIS metal product conversion to precursor oxide for light water power reactor fuel was completed. To assure integration of U-AVLIS into the nuclear fuel cycle, interactions with converter, metal maker, and fuel fabricator industries were continued.

Keywords: Enrichment, Uranium, Laser Isotope Separation, Uranium-Atomic Vapor Laser Isotope Separation (U-AVLIS)

## Office of Civilian Reactor Development

## Office of Advanced Reactor Programs

## Division of High Temperature Gas-Cooled Reactors

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

Materials Preparation, Synthesis, Deposition, Growth or Forming

253. Fuel Process Development FY 1990 $300,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. F. Turner, (619) 455-2306

This work includes establishing, characterizing, and qualifying fabrication processes and equipment for the preparation of microsphere fuel particles of uranium-oxycarbide (UCO) coated with layers of pyrolytic carbon (2) and silicon carbide (1). Major processing operations include solution mixing, kernel forming, drying, calcining, and sintering. Coatings are applied in a fluidized-bed furnace at temperatures up to 1600 °C. The objective is to develop kernel fabrication and coating specifications, which yield very low fractions of defective particles. This work also includes development of the process for fabricating the fuel compacts (short rods).

Keywords: Fuel, Ceramics, Sintering, Coatings, Chemical Vapor Deposition

Materials Properties, Behavior, Characterization or Testing

254. Fuel Materials Development FY 1990 $260,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. F. Turner, (619) 455-2306

This work includes development of the technology base required to design, qualify, and license the fuel systems for near-term steam cycle and advanced process heat HTGRs. These efforts are focused on the low enriched uranium-oxycarbide/thorium-oxide fuel system. Major elements of the work include the preparation and evaluation of irradiation specimens, development and verification of fuel performance models, and preparation and updating of fuel specifications and a design data manual.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

255. Fuel Development and Testing FY 1990 $2,100,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: M. J. Kania, (615) 576-4856

This work supports development of the technology base required to design, qualify, and license the fuels systems for near-term steam cycle and advanced process heat HTGRs. These efforts are focused on the low-enriched uranium-oxycarbide/thorium-oxide fuel system. Major elements of the work include services associated with the design, assembly, and irradiation of fuel capsules, and post-irradiation examination work in support of qualification and licensing of the reference fuel system. This work also includes support of International Cooperatives with West Germany and Japan, and a fuel test program in the French CEA COMEDIE Test Facility.

Keywords: Fuel, Ceramics, Coatings, Microstructure, Radiation Effects, Diffusion, High Temperature Service

256. Graphite Development FY 1990 $50,000

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

This work supports the evaluation and qualification of graphite materials for applications in HTGRs. Major goals of this work are to develop high strength graphites with sufficient stability under irradiation to be qualified for core components, and with sufficient oxidation resistance to be qualified for core support components. The major element of this work is the development of graphite materials test specifications and failure criteria required for reliable design analyses.

Keywords: Graphite, Ceramics, Irradiation Effects, Strength, Corrosion, High Temperature Service

257. Graphite Development and Testing FY 1990 $250,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: T. D. Burchell, (615) 576-8595

This work includes the selection, characterization, and qualification of graphite materials for applications in HTGRs. These efforts are focused on the development of fundamental understanding of the behavior of graphite under representative HTGR environmental and loading conditions. Major goals of this work are to develop high strength graphites with sufficient stability under irradiation to be qualified for core components, and with sufficient oxidation resistance to be qualified for core support components. The major elements of this work include characterization of the mechanical, physical, and chemical properties of candidate graphites and determinations of the effects of irradiation on mechanical and physical properties.

Keywords: Graphite, Ceramics, Irradiation Effects, Strength, Corrosion, High Temperature Service

258. Metals Technology Development — FY 1990 $30,000

DOE Contact: J. E. Fox, (301) 353-3985
GA Technologies Contact: R. F. Turner, (619) 455-2306

This work includes activities to characterize and qualify the metallic materials selected for applications in the HTGR system. Tasks involve work to establish the database required for design validations and code qualifications. Principal alloys include SA508 and 533 steels, 2¼ Cr-1 Mo steel, and Alloy 800H.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

259. Structural Materials Development — FY 1990 $340,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: P. L. Rittenhouse, (615) 574-5103

This work includes testing activities to characterize and qualify the metallic materials selected for application in HTGR components and structures. The emphasis of the work is to provide design data or components which operate in the primary coolant circuit, where the service temperatures are the highest and the materials may be adversely affected by trace amounts of impurities in the helium coolant. The primary testing activities include evaluations of the effects of extended high temperature exposures in simulated helium and air environments on mechanical properties and the effects of irradiation on the nil-ductility transition temperature.

Keywords: Alloys, Strength, Corrosion, Joining, Microstructure, High Temperature Service

260. Advanced Gas Reactor Materials Development FY 1990
$100,000

DOE Contact: J. E. Fox, (301) 353-3985
ORNL Contact: O. F. Kimball, (615) 574-8258

This work includes testing and evaluation of the high temperature alloys required for applications in advanced HTGRs that will operate at temperatures about 750 °C. The primary activity is operation of a testing laboratory specifically designed for extended high temperature exposures of mechanical property specimens and corrosion samples in simulated helium reactor environments. Major work elements include mechanical property and corrosion testing of commercial available and developmental candidate alloys and the generation of a database for development of high temperature design criteria and code qualification rules.

Keywords: High Temperature Alloys, Mechanical Properties, Corrosion

Office of Technology Support Programs (LMRs)

The applied research and development technology activities, conducted at several national laboratories, industrial organizations, universities, and through bilateral and trilateral technology programs and exchanges with foreign nations, relate to current and advanced reactor systems. The scope of these activities include the following areas: fuel cycles; design and performance of high quality core components for fuels, blanket, and control systems; development of the structural materials used in these components and systems; development and demonstration of equipment, processes, and procedures for fabricating, processing, handling, and producing mixed oxide bearing fuels, binary and ternary metal fuels, materials, and components; sodium technology; standards and quality assurance; assuring a reliable high quality economical fuel supply for LMRs; destructive and nondestructive testing, examination, and evaluation of core components and the facilities and capabilities for conducting such examinations; responsibility for engineering and supporting facilities; associated safety, safeguards, and nonproliferation; maintaining competent capabilities in the several contractor organizations that conduct the pertinent R&D activities and programs. These activities are responsive to the administration's policies and goals and, to the DOE programs that support them.

In-reactor and out-of-reactor property evaluations are being conducted on core materials, clad/ducts, fuels and absorber materials. Through irradiation testing in FFTF and EBR-II, the Technology Support Programs are developing, qualifying, and verifying the use of reference, improved and advanced mixed oxide and metal fuels and boron carbide absorbers, including full-size driver and blanket fuels, and absorber element pins and assemblies--same for carbide fuels. Fabrication development, evaluation, qualification, and verification (raw material processing, melting, hot working, cold working, and finishing) are conducted on reference, improved, and advanced alloys including in-reactor qualification of pins, ducts, and assemblies.

Improved and advanced materials are being tested for use in future cores. The testing for these programs is primarily conducted at government laboratories: Argonne National Laboratory at Chicago, Illinois and Idaho Falls, Idaho; Oak Ridge National Laboratory at Oak Ridge, Tennessee; and Westinghouse Hanford Company at Richland, Washington.

Fuels and Core Materials

Materials Properties, Behavior, Characterization or Testing

261. Fuel Performance Demonstration

FY 1990
$5,441,000

DOE Contact: Andrew C. Millunzi, (301) 353-3405/FTS 233-3405
ANL Contact: Leon C. Walters, (208) 526-7384/FTS 583-7384

Establish U-Pu-Zr fuel fabrication process, irradiation performance characteristics and high burn-up capability. EBR-II lead test achieved 17.1 and 18.4 a/o burn-up and were removed for PIE. Program plans to complete initial off-normal testing in EBR-II, including RBCB and fabrication variable tests.

Keywords: Breeder Reactor, Actinides, Fuel

262. Pyroprocess Development

FY 1990
$4,262,000

DOE Contact: Eli I. Goodman, (301) 353-2966/FTS 233-2966
ANL Contact: James E. Battles, (312) 972-4538/FTS 972-4538

Establish technical feasibility of the proposed pyroprocesses including electrorefining, chemical reduction, and waste treatment processes. Program will complete selection of optimum cathode configuration for electrorefining process, conduct engineering scale (10 kg) demonstration of electrorefining with uranium, and run laboratory-scale demonstration of waste treatment processes. Process optimization and development of a commercially applicable flow sheet will be started.

Keywords: Waste Treatment, Electrorefining, Pyroprocesses

263. Fuel Safety Experiments and Analysis FY 1990
$3,187,000

DOE Contact: Philip B. Hemmig, (301) 353-3579/FTS 233-3579
ANL Contact: John Marchaterre, (312) 972-4561/FTS 972-4561

Conduct analyses and experiments required for the demonstration of the safety performance of metallic fuel in fast reactor systems. Include transient fuel behavior, validated models and codes which describe fuel behavior, and safety mechanisms which contribute to inherent safety. Program will initiate analysis of high plutonium fuel to expand the data base pertaining to safety margins, failure thresholds, and transient behavior.

Keywords: Reactor Safety, Actinides, Fuel

264. Core Design Studies FY 1990
$947,000

DOE Contact: Philip B. Hemmig, (301) 353-3579/FTS 233-3579
ANL Contact: D. C. Wade, (312) 972-4858/FTS 972-4858

Provide direct support in developing optimized metallic core designs for ALMR and establish a validated design and safety analysis methodology suitable for initiation of detailed design and for licensing interactions. Conduct studies of fuel management strategies for the closed fuel cycle, including physics and economic impacts of self-sufficient uranium start-up versus maximized ratio start-up of sequential plant modules. Emphasize actinide self-consumption in the IFR metal fuel cycle to support the overall IFR waste management strategy.

Keywords: Actinides, Reactor Design, Breeding Ratio, Metal Core

265. Fuel Cycle Studies FY 1990
$3,674,000

DOE Contact: Eli I. Goodman, (301) 353-2966/FTS 233-2966
ANL Contact: M. J. Lineberry, (312) 972-7434/FTS 972-7434

Provide for start-up of fuel cycle comprehensive remote operations demonstration including completion of equipment in FCF and start-up with irradiated fuel. Proceed to fabrication of first recycled U-Zr fuel assembly. Quantify the ultimate fuel cycle economics through development of commercial fuel cycle facility design and cost estimates.

Program will continue equipment development activities for remotized in-cell application, including reusable mold concept for injection-casting furnace, semi-automated pin processor, engineering-scale pyroprocessing equipment, etc. Refine and update commercial-scale fuel cycle facility design and cost estimates, including sensitivities to throughput requirements and develop initial set of prototype equipment systems.

Keywords: Fuel, In-Cell, Remotized, Injection-Casting

266. <u>LMR Technology R&D</u> — <u>FY 1990</u> $1,345,000

DOE Contacts: Philip Hemmig, (301) 353-3579/FTS 233-3579 and C. Chester Bigelow (Seismic), (301) 353-4299/FTS 233-4299
ANL Contact: D. C. Wade, (312) 972-4858/FTS 972-4858

Continue seismic analyses and test support for the ALMR design.

Keywords: Seismic Tolerance, Enhanced Reactor Safety, Inherent Safety Features, Fuel

<u>Structural Materials and Design Methodology</u>

<u>Materials Properties, Behavior, Characterization and Testing</u>

267. <u>Structural Design/Life Assurance Technology</u> — <u>FY 1990</u> $ 0 (Funded by JAPC)

DOE Contact: Andrew C. Millunzi, (301) 353-3405/FTS 233-3405
ORNL Contact: Jim Corum, (615) 574-0718/FTS 624-0718

Program was to develop the structural design methods and criteria for use of modified 9 Cr-1 Mo steel in liquid metal reactor environment; however, it has been closed out in FY 1990. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

Keywords: Fatigue, Failure Testing, Joining and Welding, Creep

268. Modified 9 Cr-1 Mo Steel Design Properties

FY 1990
$ 0
(Funded by JAPC)

DOE Contact: Andrew C. Millunzi, (301) 353-3405/FTS 233-3405
ORNL Contact: Phil Rittenhouse, (615) 574-5103/FTS 624-5103

The program had been conducting long-term thermal aging effects on mechanical properties, long-term creep-rupture tests on base and weldment materials, creep-fatigue tests in air and high vacuum environments and creep-crack propagation tests on modified 9 Cr-1 Mo steel. The program is now supported under a DOE/Japanese exchange agreement, funded jointly by DOE and Japanese Atomic Power Company (JAPC).

Keywords: Creep, Fatigue, Tensile Testing, Toughness

269. MOTA Fabrication and Operation

FY 1990
$1,200,000

DOE Contact: Andrew C. Millunzi, (301) 353-3405/FTS 233-3405
WHC Contact: Ray J. Puigh, (509) 376-3766/FTS 444-3766

Complete activities on providing a known and controlled environment for materials irradiation tests in FFTF. Complete tests on HT9 irradiation supporting Series III fuel design, international tests, FFTF structural materials surveillance, and non-LMR tests. Upon discharge of MOTA from FFTF, examine specimens and reconstitute all samples into a new MOTA vehicle during the reactor outage if time permits. Monitor and document the operations of MOTA. Issue MOTA 1F operations report. Initiate phase out of the program in FY 1990.

Keywords: Irradiation, Environmental Testing

270. Absorber Development

FY 1990
$1,000,000

DOE Contact: C. Chester Bigelow, (301) 353-4299/FTS 233-4299, Andrew C. Millunzi, (301) 353-3405/FTS 233-3405
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Complete activities in support Series III control rod design and monitor ongoing FFTF absorber tests. This includes completing post-irradiation examination of HEHB and ADVAB-1B experiments and providing analytical support to extend FFTF absorber lifetime to 900 Effective Full Power Days (EEPD) and longer. Provide a report on absorber performance to date in FFTF. Initiate phaseout of the program in FY 1990.

Keywords: Control Rods, Nuclear Absorbers

271. FFTF Metal Fuel Testing FY 1990
$3,800,000

DOE Contact: Andrew C. Millunzi, (301) 353-3405/FTS 233-3405
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Complete FFTF metal fuel irradiations and transient testing in TREAT. Complete irradiation of FFTF binary metal driver fuel test assemblies at nominal fuel conditions (MFF-4, -5, and -6) and at 2-sigma hot channel conditions (MFF-3). Initiate phaseout of the program in FY 1990.

Keywords: Fuel, Non-ferrous Metals

272. Core Demonstration Experiment (CDE) FY 1990
$1,000,000

DOE Contact: Jacob Glatter, (301) 353-3921/FTS 233-3921
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Complete Core Demonstration Experiment (CDE) irradiation in FFTF supporting the extension of fuel lifetime to 1,200 EFPD. Complete Cycle 10 CDE report, evaluate data for justifying continued irradiation of CDE beyond goal exposure (1200 EFPD) based on steady-state and transient data. Evaluate high exposure HT9 data and report.

Keywords: Fuel, Non-ferrous Metals

273. International Collaboration FY 1990
$500,000

DOE Contact: Jacob Glatter, (301) 353-3921/FTS 233-3921
WHC Contact: Alan E. Waltar, (509) 376-5514/FTS 444-5514

Irradiate and complete DSF-1 fuel test with cladding types agreed to with DOE and PNC. Complete monitoring irradiation performance in FFTF of PNC fuel (MFA-1 and -2) and blanket (MBA-1) assemblies. Characterize and report on production lots of MA957 cladding. Irradiate MOTA NAM-1 test specimens. Initiate phase-out in FY 1990.

Keywords: Dispersion Strengthened Ferritic (DSF), Fuel, Cladding

Office of Space and Defense Power Systems

The Office of Space and Defense Power Systems responsibilities include the development, system safety and production of radioisotope powered thermoelectric generators (RTG) and dynamic power systems for NASA and DOD space and terrestrial applications and advancing base technologies for these power systems. Thus, applied materials research programs are supported in the areas of thermoelectric materials and devices, high temperature heat source materials, materials systems compatibility and safety related materials characterization and testing.

Materials Preparation, Synthesis, Deposition, Growth or Forming

274. Development of Improved Thermoelectric Materials for Space Nuclear Power Systems

FY 1990
$300,000

DOE Contact: W. Barnett, (303) 353-3097
Iowa State University, Ames Laboratory Contact: B. Beaudry, (515) 294-1366

The prime objective of this program is to apply and exploit the capabilities of the mechanical alloying process for the development of improved performance Si-Ge type thermoelectric materials. The goal or target properties are average Figure of Merits, Z of 0.8 and 1.2 x $10^{-3}$/ °C over the temperature range 300 to 1000 °C for "P" and "N" type materials, respectively.

During 1990 major emphasis was placed on developing techniques. Methods were developed to produce "N" type Si-Ge material exhibiting thermoelectric properties equal or slightly superior to that of standard Si-Ge material. Studies of alloy and process variants were initiated. Mechanical alloying continues to show excellent promise.

Keywords: Mechanical Alloying, Consolidation of Powder, Powder Synthesis, Semiconductors, Thermoelectrics

275. Development of an Improved Process for the Manufacture of DOP-26 Tridium Alloy Blanks and Exploratory Alloy Improvement Studies

FY 1990
$590,000

DOE Contact: W. Barnett, (303) 353-3097
RNL Contact: E. K. Ohriner, (615) 574-8519

An iridium alloy, DOP-26 (i.e., Ir-0.3 wt.% W with Th and Al dopant additions), serves as the fuel clad or capsule material for isotope heat sources employed in recent and contemporary space power systems for NASA deep space missions such as Voyager, Galileo and Ulysses. This program is aimed at the development of an improved process route for the production of DOP-26 iridium alloy sheet, namely a consumable arc cast/extrusion/"warm" rolling route. Thermomechanical process parameters shall be optimized with respect to uniformity of product grain morphology, high strain rate, high temperature ductility and formability. The product must meet or exceed existing DOP-26 iridium alloy specifications.

It is anticipated that the DOP-26 alloy 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).

Also, exploratory iridium alloy development studies were initiated with the goal of improved weldability and enhanced thermal stability and high strain rate ductility relative to the state of the art DOP-26 alloy.

During FY 1990 production procedures were established for the consumable arc melt/ extrusion route process for DOP-26 alloy sheet, blanks and foil. A production readiness review was successfully completed. Initial production results indicate the goal of improved process yields will be met. A "requal program" for this new product is in the planning stage.

Installation of a new consumable arc melting furnace was 90 percent completed. Acceptance testing at the vendor's (Leybold-Heraeus) shop of a new electron beam melting furnace was successfully completed in September, 1990, with delivery scheduled for the 4th quarter. Qualification of these major capital improvements for production use if planned for 1991.

Exploratory alloy development activities were aimed at the study of alternate dopants to the thorium used in the DOP-26 alloy. Preliminary results suggest that cerium is a promising candidate.

Keywords: Consumable Arc Melt, Extrusion, Noble Metal

276. <u>Carbon Bonded Carbon Fiber Insulation Manufacturing Process Development and Product Characterization</u>

FY 1990
$ 0

DOE Contact: W. Barnett, (303) 353-3097
ORNL Contact: R. L. Beatty, (615) 574-4536

Carbon-bonded carbon fiber (CBCF) type thermal insulation material is employed in Isotopic General Purpose Heat Source (GPHS) Module assemblies for use in current GPHS-RTG (radioisotope thermoelectric generator). The GPHS RTGs power the spacecraft for the NASA Galileo and NASA/ESA Ulysses missions and will be employed for the 1995-1996 NASA CRAF and Cassini missions. This CBCF process development program is intended to accommodate a replacement carbon fiber (present specified fiber is no longer available), improve process controls, and optimize process parameters. The product shall meet prior flight quality CBCF specification. Product characterization shall include chemical purity, density, compressive strength, and thermal conductivity.

During 1990 process optimization was completed. Production procedures were updated as a production readiness review was successfully completed. Production of CBCF sleeve/disc sets was initiated and 30 units were completed.

Keywords: Insulators/Thermal, High Temperature Service, Fibers

Device or Component Fabrication, Behavior or Testing

277. Nondestructive Testing Methods Development and Application to Thermoelectric Materials and Devices

FY 1990
$110,000

DOE Contact: W. Barnett, (303) 353-3097
ORNL Contact: B. E. Foster, (615) 574-4837

Continued support program aimed at the development and application of state-of-the-art nondestructive examination (NDE) techniques for Si-Ge thermoelectric materials, multicouples and multicouple subassemblies. Particular attention was directed toward the evaluation of glass bonds and hot shoe bonds, and the post-test diagnostic evaluation of multicouples.

Support was provided to General Electric Company, Valley Forge, Pennsylvania, in their development of the MOD-RTG multicouple.

Keywords: NDE, Semiconductor Devices, Thermoelectrics

Materials Properties, Behavior, Characterization or Testing

278. Characterization of State-of-the-Art Improved Silicon-Germanium Thermoelectric Device/Materials

FY 1990
$150,000

DOE Contact: W. Barnett, (303) 353-3097
Iowa State University Contact: B. Beaudry, (515) 294-1366

This program is concerned with the evaluation and characterization of state-of-the-art Si-Ge/GaP and other "improved" silicon-germanium type thermoelectric materials. Also, the compatibility of materials, both current and candidates, employed in the manufacture of the multicouple (i.e., glass bonded close packed arrays of silicon-germanium couples) device are to be studied.

The isothermal aging response of MOD-RTG "N" type Si-Ge/GaP and "P" type Si-Ge materials was evaluated over the temperature range 400-1000°C for times of up to 80,000 hours. Studies of various cold and electrical contact systems for Si-Ge type alloy were initiated using diffusion bonding techniques. Tungsten has shown attractive characteristic.

Keywords: Semiconductor, Thermoelectrics, Diffusion Bonding, Electrical Contacting

279. <u>Development of an Improved Carbon-Carbon Composite Graphite Impact Shell Replacement Material</u> <u>FY 1990</u>
$185,000

DOE Contact: W. Barnett, (301) 353-3097
Oak Ridge National Laboratory Contact: M. Martin, (616) 574-4351

The Graphite Impact Shell (GIS), a component of the General Purpose Heat Source isotopic heat source module is a closed end/capped tubular shape machined from AVCO 3D-CC fine weave pierced fabric material. It is anticipated that a change in the fiber reinforcement architecture from the current orthogonal structure to a cylindrical type structure will enhance energy absorption in high velocity impact. The current program is a feasibility study of commercially available materials.

During 1990 a survey of commercially available materials was conducted and their relative merits were assessed. Two different reinforcement architectures were selected and procurement of test materials was initiated.

Keywords: Composite, Carbon-Carbon

<u>Office of Naval Reactors</u>

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 $88 million in FY 1990 including approximately $48 million as the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Robert H. Steele, (703) 603-5565/FTS 283-5565.

# OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

## Office of Civilian Radioactive Waste Management/Yucca Mountain Site-Characterization Project Office (OCRWM/YMPO)

The primary goal of the OCRWM/YMPO materials program is the development of tuff-specific waste packages that meet the NRC's performance requirements. This work includes the definition of physical and chemical conditions of the site, evaluation of the package materials, waste package design and performance assessment, prototype waste package fabrication, and performance testing. (As a result of the Nuclear Waste Policy Act Amendments, the Salt Repository Project and the Basalt Waste Isolation Project were terminated effective March 1989.)

### Materials Properties, Behavior, Characterization or Testing

280. Waste Package Environment — FY 1990 $1,663,000

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the time-dependent behavior of the hydrogeologic, geochemical and mechanical 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

281. Waste Form Testing — FY 1990 $3,463,900

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the behavior of and determine the radionuclide release rates for the various waste forms in the geological tuff environment and as modified by corrosion products in the "Metal Barrier Testing" and "Other Engineering Barrier Waste Package Components" results. This includes work on both borosilicate glass and spent fuel.

Keywords: Radioactive Waste Host, Materials Degradation

282. Metal Barrier Testing FY 1990 $1,953,500

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the behavior of and determine the degradation modes and rates for candidate metallic barrier materials in the environment. This information is needed to establish the data base to support license applications predictions of containment of radioactivity for times required by NRC 10 CFR 60. Characterize the properties and behavior of other engineered barrier waste package components that may be present in a repository.

Keywords: Materials Degradation, Radioactive Waste Host

283. Other Engineered Barrier/Waste Package Components FY 1990 $ 0

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the properties and behavior of other engineered barrier and waste package components that may be present in a repository. This information is needed to establish the predicted performance of other materials, such as non-metallic barrier materials or 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

284. Integrated Testing FY 1990 $1,950,400

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Characterize the integrated behavior of the waste form, barrier materials, and surrounding environment. Determine thermodynamic properties of Actinide and fission products.

Keywords: Actinide Chemistry, Waste Package Testing, Thermodynamic Data Base

285. Waste Package: Performance Assessment FY 1990 $986,500

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Provide a quantitative prediction of long-term waste package performance. This information, including uncertainties, is needed to provide feedback to design optimization studies, to demonstrate compliance with NRC performance objectives for the Waste Package Subsystem, and to provide a source term for the Engineered Barrier System and the Total System performance assessments required by NRC 10 CFR 60 and EPA 40 CFR 191.

Keywords: Waste Package Performance, Uncertainty Analysis

286. Research on Geochemical Modeling of Radionuclide Interaction with a Fractured Rock Matrix FY 1990 $1,057,600

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Further develop the geochemical modeling code EQ3/6 for use in long-term predictions of radionuclide release from a nuclear waste repository.

Keywords: Geochemical Modeling, Computer Modeling, Rock-Water-Waste Interaction

Device or Component Fabrication, Behavior or Testing

287. Waste Package: Design, Fabrication and Prototype Testing FY 1990 $697,700

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Develop, analyze, fabricate, and test waste package designs that incorporate qualified materials which are fully compatible with the repository design. This work supports license application by demonstrating conformance with requirements for safe handling, emplacement, possible retrieval, and credible accident conditions per NRC 10 CFR 60 and EPA 40 CFR 191 in a cost-effective manner.

Keywords: Radioactive Waste Package Development

288. Waste Package Environment Field Tests

FY 1990
$867,500

DOE Contact: C. P. Gertz, (702) 794-7920
LLNL Contact: David Short, (415) 422-1287

Develop a detailed engineering test plan for the waste package environment in situ testing program and evaluate, design, fabricate, and test thermomechanical and hydrologic instrumentation for waste package in situ test measurements. 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.

Keywords: Radioactive Waste Packaging Tests, Instrumentation and Technique Development, Field Testing

# 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 Research and Advanced Technology and in the Office of Nuclear Materials Production. Within the Office of Research and Advanced Technology, materials activities are supported by the Inertial Fusion Division and by the Research and Technology Development Division.

<u>Office of Research and Advanced Technology</u>

<u>Research and Technology Development Division</u>

<u>Sandia National Laboratories - Albuquerque</u>

<u>Solid State Sciences Directorate, 1100</u>

<u>Ion Solid Interactions and Surface Sciences Research Department, 1110</u>

The mission of Department 1110 is to provide Sandia National Laboratories with a comprehensive research program and technology base in the surface and interface science ion implantation, ion-solid microanalysis/channeling thin film kinetics and epitaxy, and defects and hydrogen in solids. The research is designed to enhance fundamental understanding of the physical and chemical processes necessary to control the near-surface and interfacial regions of solids as well as to develop new techniques for the controlled synthesis, modification and analysis of these near-surface and interfacial regions. A major aspect of the work is thus to develop an underlying understanding and control of defects, thin film kinetics, epitaxy, hydrogen-materials interactions alloying processes, and the formation of metastable and amorphous phases. In addition, the mission of the department is to relate this knowledge to laboratory problems and needs in the development of advanced weapons and energy systems.

Materials Properties, Behavior, Characterization or Testing

289. Ion Implantation Studies for Friction, Wear and Microhardness FY 1990
$300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL (Contract No. DE-AC04-76DP00789) Contacts D. M. Follstaedt, (505) 844-2102, S. M. Myers, (505) 844-6076 and L. E. Pope, (505) 844-5041

Ion implantation is used to modify the surface and near-surface regions of metals, and these implantation-modified materials are evaluated for their improved friction and wear characteristics. Of particular interest is the implantation of Ti + C into bearing steels to concentrations sufficient to form amorphous layers in the near-surface region. These amorphous layers have been found to yield significantly improved friction and wear behavior for steels, independent of the structure and composition of the starting material. Extensions of these studies to vacuum applications are under investigation. A second area is the formation of ultrahard and stable Al alloys by oxygen implantation.

Keywords: Ion Implantation, Friction, Wear, Amorphous Metals

290. Silicon-Based Radiation Hardened Microelectronics FY 1990
$670,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL (Contract No. DE-AC04-76DP00789) Contacts: H. J. Stein, (505) 844-6279, B. L. Doyle, (505) 844-2609 and J. A. Knapp, (505) 844-2305

Optical, electrical and compositional measurements, in conjunction with electron paramagnetic resonance, Rutherford backscattering/channeling, and related techniques are used to determine the fundamental defect structures and materials properties required for radiation-hardened Si-based microelectronics. Recent studies have concentrated on amorphous silicon nitride, which is the charge storage medium for radiation-hard nonvolatile semiconductor memories; defects in $SiO_2$ and at the Si-$SiO_2$ interface, which markedly affect the radiation tolerance of MOS devices, and the formation of buried dielectric layers which may be essential for next generation radiation hard microelectronics. Relationships between the materials composition, chemical bonding, and defect configurations and the electrical performance are evaluated to permit long-term prediction of the performance of devices in a radiation environment and to develop new structures with particular properties.

Keywords: Microelectronics, Radiation Hardened, Silicon Nitride, Silicon, Silicon Dioxide, Defects

291. Surface Science FY 1990
$400,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: T. A. Michalske, (505) 844-5829

Scanning tunneling microscopy, field ion microscopy, Auger electron spectroscopy, synchrotron and lab-based UV photoemission spectroscopy, and thermal desorption are being used to understand at an atomic level the early stages of epitaxy, oxidation and corrosion of metals and semiconductors, the nature of the adhesion of polymers to metals and how to improve it, and the formation of interface states and fine structures. Novel chemical vapor deposition techniques are being developed to explore formation of more uniform and reliable high temperature coatings.

Keywords: Surface Physics, Scanning Tunneling Microscopy, Field Ion Microscopy, Auger Electron Microscopy, UV Photoemission Spectroscopy, Oxidation, Corrosion, Adhesion

Laser and Chemical Physics Research Department, 1120

Materials processing science studies emphasizing chemical vapor deposition and plasma- and photo-enhanced chemical vapor deposition and etching are carried out. Emphasis is on microelectronic and optoelectronic materials and processing methods. Examples of ongoing studies include:

Materials Properties, Behavior, Characterization or Testing

292. Plasma Etching FY 1990
$500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

Optical diagnostics are emphasized in fundamental studies of plasmas of the type widely used in the manufacture of large-scale and very-large-scale integrated electronic circuits to etch small features in semiconductors, dielectrics and conductors. Emphasis is placed on gaining improved understanding of the underlying physics and chemistry of technologically-important processes occurring both in the volume and on the surface. The goal of this study is the development of new process methods and methodologies that give improved pattern-transfer fidelity and less damage to the underlying material. A secondary goal is the development of process monitors that may lead to improved process reliability.

Keywords: Plasma Etching, Microelectronics

293. Plasma-Enhanced Chemical Vapor Deposition — FY 1990 $100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: K. E. Greenberg, (505) 844-1243 and P. J. Hargis, (505) 844-2821

Optical diagnostics are emphasized in fundamental studies of plasma-enhanced chemical vapor deposition, PECVD, of thin-film materials of the type that are used in the manufacture of microelectronic devices. Plasma-enhanced CVD offers advantages in comparison to thermal CVD in that high-quality materials can be deposited at lower temperatures. Lower-temperature processing offers latitude in device fabrication, especially as to how a particular fabrication step may affect the properties of materials that were defined in previous process steps. The goal of these studies is to develop processes that give higher quality materials having good adhesion to the underlying structure. A secondary goal is to develop *in situ* monitors for process control.

Keywords: Plasma Deposition, Microelectronics, Chemical Vapor Deposition

294. Laser-Controlled Etching and Deposition of Materials — FY 1990 $250,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: A. Wayne Johnson, (505) 844-8782

We are studying the underlying science and the technological limits of laser-controlled deposition and etching of conductors and insulators on microelectronic circuits. This technology is expected to find important applications for the correction of design errors in prototype circuits and for customization of large-scale integrated circuits.

Keywords: Laser Etching, Laser-Induced Chemistry, Microelectronics

295. Surface Chemistry of Organometallics for Compound Semiconductor Epitaxy

FY 1990
$300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: J. R. Creighton, (505) 844-3955

The motivation for this study stems from the extensive use of organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc.) as sources of elemental constituents for the growth of compound semiconductors by such techniques as metallorganic chemical-vapor deposition (MOCVD) chemical-beam epitaxy (CBE), and atomic layer epitaxy (ALE). Technology is leading science in these important compound semiconductor growth processes, and our lack of a detailed understanding of the underlying physics and chemistry, especially surface chemistry, is hindering advances necessary to produce future generations of optoelectronic materials and devices. Breakthroughs in understanding the underlying surface chemistry require a break from conventional methods of trial and error system optimization. Here we probe the primary chemical surface reactions to gain a scientific understanding of these technologically important systems. With the emergence of new understanding, higher quality materials should follow.

Keywords: Surface, Deposition, Epitaxial Growth, Chemical Vapor Deposition

296. Metallorganic Chemical Vapor Deposition

FY 1990
$500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: K. P. Killeen, (505) 844-5164 and M. E. Coltrin, (505) 844-7843

The deposition of thin films of III-V compound semiconductor materials to produce scientifically tailored semiconductor structures is often done by thermal chemical vapor deposition using Group III organometallic compounds ($Ga(CH_3)_3$, $Al(CH_3)_3$, etc., and Group V hydrides ($AsH_3$, $PH_3$, etc.) or alkyls ($As(CH_3)_3$, $P(C_2H_5)_3$, etc.). The control of these technologically important processes to give quality material is an art with little scientific foundation. In this program we are applying comprehensive theoretical modelling of the fluid dynamics and both the volume and the surface chemistry, as well as an extensive array of *in situ* measurement tools to gain new insight into the underlying physics and chemistry of the process. The goal of this work is the development of processes and process-control procedures that yield higher quality materials and more abrupt heterointerfaces. Another objective of the work is to identify chemical precursors that are less toxic and otherwise more safe to handle.

Keywords: Chemical Vapor Deposition, Process Modelling, Thin Films

Compound Semiconductor and Device Research Department, 1140

Study and application of semiconductor strained-layer superlattices and heterojunction materials to explore solutions to new and existing semiconductor materials problems by coordination of semiconductor physics (theory and experiment) and materials science. This program investigates fundamental material properties including band structure, electronic transport, crystal stability, and linear and nonlinear optical properties. It also includes investigation of thin film high temperature superconductors for hybrid compound semiconductor/superconductor applications. The materials under study have a wide range of applications for high speed and microwave technology, optical detectors, lasers, and optical modulation and switching.

Materials Preparation, Synthesis, Deposition, Growth or Forming

297. Materials Growth by Molecular Beam Epitaxy (MBE) FY 1990 $500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contacts: L. R. Dawson, (505) 846-3451, T. M. Brennan, (505) 844-3233 and J. F. Klem, (505) 844-9102

Growth of AlGaAs/GaAs, InAsSb/InAl, InGaAs/GaAs and AlInAs/GaInAs strained layer superlattice (SLS) and strained quantum well (SQW) structures for electronic and optoelectronic applications. These structures are either uniformly doped for application in a typical electronic device or modulation doped for novel device structures, including high speed electronic devices, light emitting diodes and detectors.

Keywords: Semiconductor Device Fabrication, Strained Layer Superlattices, Strained Quantum Well

298. Materials Growth by MOCVD FY 1990 $400,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
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

299. Strained Layer Superlattices for IR Detectors FY 1990 $300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contacts: S. R. Kurtz, (505) 844-5436 and L. R. Dawson, (505) 846-3451

Strained layer superlattices based on the InAsSb/InSb and InAsSb/InSb/AlSb systems are being investigated for use as attractive alternatives to the unstable HgCdTe alloys for IR detector applications in the 8-12 $\mu$m range. These IR materials are being grown by both MBE and MOCVD techniques and evaluated by electrical and optical techniques. Photovoltaic detectors with $D^* > 1 \times 10^{10}$ cm $\sqrt{HZ/W}$ at 10 $\mu$m and 77K and photoconductive detection to 15 $\mu$m have been demonstrated.

Keywords: Strained-Layer Superlattices, Infrared Detectors

300. Novel Processing Technology for Semiconductor Technologies FY 1990 $500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contact: D. S. Ginley, (505) 844-8863.

This program involves studies of new technologies for formation of diffusion barriers for improved epitaxial growth, novel metallurgies for Shottky barrier and Ohmic contact formation, passivation layer development, and development of new metallurgical techniques for deposition of reactive alloys, and deposition and patterning of high temperature superconductors to interconnects on semiconductor devices.

Keywords: Semiconductor Devices

301. Thin Film Superconductors

FY 1990
$300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contact: D. S. Ginley, (505) 844-8863

Thin films of the high temperature superconductors in the Y-Ba-Cu-O and Tl-Ca-Ba-Cu-O systems are being prepared by MBE, E-beam evaporation and sputtering. Oriented and random films with $T_c$s to 112K are being produced. Strongly-linked polycrystalline films with critical currents approaching 1,000,000 A/cm $^2$ at 77K have been demonstrated. Patterning and contacting technology for the films for device applications is also being developed.

Keywords: Thin Films, High Temperature Superconductors, Coatings and Films

Condensed Matter Research Department, 1150

The mission of Department 1150 is to provide fundamental understanding and strong technology bases in novel materials and structures, surface physics and shock wave physics and chemistry. Both experimental and theoretical research are performed. Current areas of emphasis include high $T_c$ superconductors, shock-induced solid state chemistry, disordered materials, high temperature semiconducting borides defects in semiconductors, surface desorption and ferroelectrics.

Materials Properties, Behavior, Characterization or Testing

302. Superconductivity

FY 1990
$650,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contact: B. Morosin, (505) 844-8169

Transport, magnetic and structural measurements to access the fundamental factors which limit the performance of ceramic superconductors. Development of theoretical models of high temperature superconductivity. Development of new processing technologies for ceramic superconductors, in particular high pressure, high temperature oxygen treatments.

Keywords: Superconductivity, Ceramics

303. Shock Physics and Chemistry FY 1990
$500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contact: R. A. Graham, (505) 844-1931

Both organic and inorganic solids are being investigated to determine the influence of molecular structure on shock-induced bond scission, and the influence of line and point defects on the observed enhanced, shock-induced solid state reactivity. Shock-induced, highly exothermic chemical reactions are being investigated for potential applications. The influence of shock modification on the properties and synthesis of high $T_c$ superconductors is being explored. Shock-activated thermal batteries are being studied to determine the mechanisms and materials parameters which influence electrical output. The work also provides insights about the nature of the shock process itself. A revolutionary time-resolved dynamic stress gauge using the piezoelectric polymer $PVF_2$ is being developed for laboratory, field testing and component diagnostics application. The mechanism for the operation of the gauge is being investigated.

Keywords: Organic Solids, Inorganic Solids, Molecular Structure, Shock, Chemical Reactions

304. Semiconductors FY 1990
$600,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contacts: D. Emin, (505) 844-3431 and H. P. Hjalmarson, (505) 846-0355

Theoretical and experimental studies of electronic properties of boron carbide at high temperatures. Radiation-induced defects and their deep electronic levels in silicon and compound semiconductors and the role of these defects in device degradation. Physics of light-hole devices based on strained layer superlattices.

Keywords: Semiconductors, Boron Carbides, Defects, Deep Levels

305. Surface Science FY 1990
$650,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contact: D. R. Jennison, (505) 844-5909

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

Keywords: Surface, Desorption, Predictive Modeling

306. Disordered Materials FY 1990
$600,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
Sandia Contact: G. A. Samara, (505) 844-6653

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

Keywords: Glass-Ceramics, Sol Gel Process, Thin Films, Microemulsions

Optoelectronics and Microsensor Research Department, 1160

The mission of Department 1160 is to provide Sandia National Laboratories with a comprehensive science and technology base in photonics and microsensor research. A fundamental understanding of the interaction of materials with both electromagnetic and mechanical forms of energy as well as their chemical environment are used to facilitate the design of new photonic and sensor devices. Activities include research into advanced materials and devices for: optical sources, modulators and detectors; information processing; and chemical sensing.

Materials Properties, Behavior, Characterization or Testing

307. New Concepts in Microsensors FY 1990
$750,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: R. C. Hughes, (505) 844-8172, A. J. Ricco, (505) 844-4907 and M. A. Butler, (505) 844-6897

New concepts in microsensors are being developed for a variety of stimuli, including radiation, magnetic fields, chemical species, and liquid-surface interactions using principles of semiconductor device operation and fabrication, surface acoustic wave propation, and optical properties of solids. Microsensors based on the properties of semiconductor surfaces include a radiation-sensing field-effect transistor (RADFET), which operates by the trapping of radiation-produced holes in the silicon dioxide gate dielectric of the FET, and chemical sensors which operate by inducing charged layers at the metal-silicon dioxide interface in response to the chemical species. Acoustic wave devices have been developed which offer new capabilities for detection and solid-liquid interface phenomena like viscosity, freezing, and low level chemical detection. Optically-based corrosion and energy impulse detectors based on the properties of new materials, like coated optical fibers, are being developed for high speed impulse detection and remote corrosive species detection. A miniature optical fiber micromirror chemical detector has been developed which can distinguish between water and common organic solvents which might be present in a contaminated toxic waste site.

Keywords: Microsensors, Microcircuitry

Materials and Process Sciences, 1800

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

308. Sulfonated Aromatic Polysulfones — FY 1990 $100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: R. L. Clough, (505) 844-3492, C. Arnold, Jr., (505) 844-8728 and R. A. Assink, (505) 844-6372

Sulfonated alpha-methyl polystyrenes are being synthesized and evaluated as chemically-stable, thin-film, cation-permeable membranes which have a large cost advantage compared with fluorinated materials. Aging and resistivity tests are continuing. Sulfonation of other high-stability polymers including polyphenylene, as well as preparation of commercial microporous membrane materials with the new cation-permeable polymers is underway. This latter work is aimed at enhancing the efficiency of commercial membrane systems.

Keywords: Polymers, Coatings and Films, Batteries

Materials Properties, Behavior, Characterization or Testing

309. Radiation Hardened Dielectrics FY 1990
$350,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: R. L. Clough, (505) 844-3492 and C. Arnold, Jr., (505) 844-8728

Polymer dielectrics are being developed that display a minimum radiation-induced conductivity (RIC). These materials will be used in capacitors and cables exposed to high dose rate radiation so that little charge is lost due to RIC in this environment. Mylar doped with an electron acceptor complex (TNF) has been shown to be a very effective rad-hard material. Studies on the aging behavior of this material are underway. A large production run on the material has been completed, and another is planned. Capacitors made from this material have been fabricated and successfully tested. A parametric study on processing conditions has been carried out, and this will lead to a formal production specification.

Keywords: Radiation Effects, Polymers, Weapons

310. Organic Nonlinear Optical Materials FY 1990
$125,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: R. L. Clough, (505) 844-3492, P. A. Cahill, (505) 844-5754, G. E. Pike, (505) 844-7562, and M. B. Sinclair, (505) 844-5506

Both second and third order organic nonlinear optical materials (dyes and polymers) are being synthesized for applications including electro-optic and photonic switching, frequency summation (through an anomalous-dispersion phase-matching process), and spatial light modulation. Some of the new materials exhibit nonlinearities an order of magnitude larger than other organic materials. Recently-initiated research on the fabrication of devices based on these materials is aimed at integrated optical devices on semiconductor substrates.

Keywords: Nonlinear, Optics, Optical, Organic, Waveguides

Physical Chemistry and Mechanical Properties of Polymers Division, 1812

Division 1812 develops new organic materials, structurally and chemically characterizes organic materials, and studies their mechanical properties. It is responsible for characterizing the molecular, electronic, and microphase structure of organic materials and their chemical reactivity toward the use environment as well as formulation of organic composites and adhesives.

Materials Preparation, Synthesis, Deposition, Growth or Forming

311. Chemistry of Plasma Etching and Deposition Processes — FY 1990 $130,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: C. L. Renschler, (505) 844-0324 and R. J. Buss, (505) 844-7494

The chemistry of glow discharge plasmas, used in a wide range of materials processing applications, is being studied with molecular beam and laser techniques. In microelectronic fabrication, the feature morphology is directly related to the detailed etch mechanism of the plasma for different materials. The interactions of plasma-generated radicals with electronic materials are being investigated to identify the significant chemistry leading to etch selectivity. Also being studied are plasma cleaning and chemical modification processes with are used extensively in weapons-component manufacture. The complex plasma chemistry determines the conditions under which the required cleaning as opposed to undesirable deposition will occur. Molecular beam and laser probing techniques are being used to identify the reactive species and their chemistry and thereby optimize the plasma processing and develop new applications.

Keywords: Plasma Etching, Plasma Deposition

Materials Structure and Composition

312. Materials Structure, Dynamics, and Property Studies by Multinuclear Pulsed NMR Spectroscopy — FY 1990 $75,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: C. L. Renschler, (505) 844-0324 and R. A. Assink, (505) 844-6392

Multinuclear nuclear magnetic resonance spectroscopy of liquid and solid samples is being applied to several materials related problems. The $^{13}C$ and $^{1}H$ spectroscopy of liquids was used to determine the molecular weight and stereochemistry of precursors used in the preparation of encapsulants and foams. The chemical structures of newly synthesized explosives were also analyzed. Both liquid and solid state spectroscopy are being applied to the study of degradation pathways and products in organic materials. Imaging techniques have been used to characterize liquid foams and will be adapted to solid foams.

Keywords: Polymers, Organics, Coatings, Coatings and Films

313. Mechanistic and Kinetic Studies of Polymer Aging — FY 1990 $250,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: C. L. Renschler, (505) 844-0324, K. T. Gillen, (505) 844-7494 and R. L. Clough, (505) 844-3492

Polymer aging under a variety of environmental stresses (e.g., thermal, radiation), is critically important in a wide range of applications. The understanding of dose rate effects is particularly important to the formulation of a predictive capability for radiation aging situations. We have developed several experimental techniques, including density and modulus profiling, to monitor the depth-dependent aging of thin polymer samples. The data obtained from these experiments have then been used to validate kinetic theory which we developed to predict oxidative aging effects in a quantitative way.

Keywords: Polymer Aging, Profiling, Kinetics

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

314. Microporous Foam Development — FY 1990 $150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: J. G. Curro, (505) 844-3963 and R. R. Lagasse, (505) 845-8333

We are developing new polymer and carbon foams which have both low density and very small cell sizes (0.1 to 10 microns). The process utilizes thermally induced phase separation followed by solvent removal steps such as extraction or freeze-drying. It has been applied to many polymers such as polystyrene, polyethylene, and polyacrylonitrile (PAN). PAN foams have many potential applications.

Keywords: Foams, Microcellular, Phase Separation, Carbon

315. Development of Removable Encapsulants — FY 1990 $30,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: J. G. Curro, (505) 844-3963, D. B. Adolf, (505) 844-4773 and P. B. Rand, (505) 844-7953

In order to allow the "rework" of expensive electronic components, a removable encapsulant is being developed. This new concept for a removable encapsulant involves infusing a blowing agent into polymer beads. The beads are a free flowing powder which can be poured into an electronic assembly. After filling, the component is heated to a temperature above the glass transition temperature of the polymer. As the polymer softens and foams, the microspheres are fused together to form a syntactic foam. The resultant syntactic foam has good compressive strength, high modulus, and a low coefficient of thermal expansion thus making an excellent encapsulant. Removal of the encapsulant for rework is easily achieved by solvent treatment. Processes are currently being developed to encapsulate large complex electronic assemblies with this material.

Keywords: Polymers, Foam, Encapsulants

Materials Properties, Behavior, Characterization or Testing

316. Mechanical Properties of Encapsulants — FY 1990 $21,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: J. G. Curro, (505) 844-3963 and D. B. Adolf, (505) 844-4773

Accurate thermophysical properties are essential as input to computer codes designed to calculate stress levels in electronic components. To date, we have measured those linear elastic properties (coefficient of thermal expansion, bulk modulus, and shear modulus) as functions of temperature that lead to stresses upon thermal cycling for common polymeric encapsulants used at Sandia. Future studies will focus on the ultimate properties of these materials for use in determining failure criteria in the computer codes.

Keywords: Polymeric Encapsulants, Organic, Tests, Bulk Modulus

317. Deformation of Kevlar Fabrics

FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: J. G. Curro, (505) 844-3963 and W. E. Warren, (505) 844-4445

The effects of weave geometry and the size, spacing and elastic properties of individual Kevlar yarns on the effective elastic response of woven Kevlar fabrics are being investigated both experimentally and theoretically. The results are important for understanding the effects of fabric structure on mechanical response. They will improve our ability to design high performance fabrics such as those required for new parachute applications.

Keywords: Fibers, Polymers, Fracture, Creep, Parachutes

Materials Structure and Composition

318. Theory of Polymer Dynamics

FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: J. G. Curro, (505) 844-0324

A number of constructs, most notably reputation and modified reputation theories (e.g., tube renewal, constraint release) have been developed in an attempt to explain the dynamics of polymer liquids (blends, melts). These theories generally begin with assumptions which are plausible, but somewhat arbitrary. More troublesome is the fact that predictions arising from these theories are often not borne out by experiment. We are developing a model of the dynamics of polymer, liquids based on microscopic statistical mechanics. This model calculates structure-property relationships from first principles with no adjustable parameters and no a priori assumptions about liquid structure or mode of motion. We anticipate eventual extension of the theory to glasses.

Keywords: Polymer Liquids, Dynamics

Electronic Property Materials Division, 1815

Division 1815 provides support to Sandia programs through selection, development, and characterization of electronic materials. Responsibilities span exploratory development through design, production, and stockpiling. The Division also performs in-depth studies in order to understand material properties and associated electronic phenomena. Areas of activity include electronic materials, dielectrics, and optical materials.

Materials Properties, Behavior, Characterization or Testing

319. Nonlinear Optical Materials FY 1990 $100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: G. E. Pike, (505) 844-7562 and M. L. Sinclair, (505) 844-5506

Measurements of refractive index and optical absorption and changes thereof are being made in organic molecules and polymers due to light or electric fields. Techniques used include attenuated total reflection from wave-guide coupling, and direct waveguide scattering.

Keywords: Nonlinear Optical, Organic

320. Hydrogen Effects in Silicon FY 1990 $50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: G. E. Pike, (505) 855-7562, R. A. Anderson, (505) 844-7676 and C. H. Seager, (505) 844-9168

Properties of silicon microelectronic devices are greatly affected by hydrogen, through a host of reactions with the silicon and its dopants. The linetics of the hydrogenation process and dopant passivation in both n- and p-type silicon is being determined, as well as hydrogen redistribution during thermal annealing. Real-time, *in situ* capacitance-voltage measurements and numerical modeling have yielded new findings; of particular significance, the dissociation of dopant-hydrogen complexes is electronically controlled.

Keywords: Silicon, Hydrogen, Dopant Passivation

321. Ferroelectric Thin Films for Nonvolatile Memories FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: G. E. Pike, (505) 844-7562, W. K. Schubert, (505) 846-6548 and W. L. Warren, (908) 975-4863

High quality, stable, ferroelectric thin films are needed for the development of new generations of microelectronic nonvolatile memories. The films must maintain low coercive field and high remanent polarization even after $10^{12}$ read/write cycles. Various electrical and electron paramagnetic resonance measurements are used to investigate the role of microstructure, impurities, and defects in determining the ferroelectric performance, and aging characteristics of $PbO$-$ZrO_2$-$TiO_2$ films.

Keywords: Ferroelectric

Materials Characterization Department, 1820

Department 1820 performs chemical analysis and materials characterization in support of weapon and energy programs and projects throughout the laboratory, and it has responsibility for the development of advanced techniques to meet anticipated needs. In addition, the department is involved in other areas such as materials compatibility, minimizing waste and certain other environmental areas.

Materials Properties, Behavior, Characterization or Testing

322. Gamma Imaging of Radioactive Waste — FY 1990 $84,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: Laura Gilliom, (505) 844-3936 and Willard Harland, (505) 844-7758

A two-dimensional imaging capability for high level radioactive waste is being developed to be used in conjunction with robots to characterize DOE wastes stored at various sights.

Keywords: Radioactive Waste

323. Diamond Coating — FY 1990 $49,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: Laura Gilliom, (505) 844-3936 and D. R. Tallant, (505) 844-3629

Raman spectroscopy is being used to characterize diamond and diamond-like films prepared in other Sandia Laboratories.

Keywords: Diamond

324. Phase Transformation in Thin Ferroelectric Films FY 1990
$72,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: Laura Gilliom, (505) 844-3936 and R. P. Goehner, (505) 844-9200

X-Ray crystallography is being used to determine the phase transformations that occur when an electric field is applied to these materials.

Keywords: Ferroelectric

325. Sensor Fabrication from Porous Silicon Using Electrochemical Techniques
FY 1990
$77,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: M. Keenan, (505) 844-2190 and M. Kelly, (505) 844-4031

Electrochemical techniques are being used to fabricate moisture sensors and to characterize defects in SOI technology. This project is joint with other Sandia organization.

Keywords: Microelectronics

326. Improved Chemometric Techniques FY 1990
$95,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: M. Keenan, (505) 844-2190 and D. Haaland, (505) 844-5292

One area of chemometrics that we are developing is the application of multivariate analysis to spectral data. We are continuing a long-term project to apply this technique to instrumental analysis of materials with particular emphasis to the identification of outliers and the transfer of the calibration model data from one instrument to another.

Keywords: Analytical Technique

327. Direct Bonding of Films and Substrate Using Ion Processing FY 1990
$59,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: J. Borders, (505) 844-8855 and A. Galuska, (505) 844-3187

High energy ion mixing is being used as a tool to better understand the mechanisms of certain thin-film bonding processes and determine improved bonding procedures.

Keywords: Joining

328. Kinetics of the Oxidation of Solder Alloys

FY 1990
$59,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: J. Borders, (505) 844-8855 and J. Nelson, (505) 846-7388

The rate of oxide growth on solder material is being determined in order to predict long-term reliability of weapon components.

Keywords: Solder, Joining

329. Segregation of Impurities to Defects in Silicon

FY 1990
$54,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: M. Carr, (505) 846-1405 and J. R. Michael, (505) 844-9115

We are developing analytical electron microscopy as a tool to analyze the extent to which impurities in silicon migrate to defects.

Keywords: Microelectronics, Semiconductors

330. Characterization of Semiconductor Materials

FY 1990
$120,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: M. Carr, (505) 846-1405 and T. Headley, (505) 844-4787

We are applying various analytical instruments to the characterization of semiconductor materials in support of research centered elsewhere in the laboratory.

Keywords: Semiconductors

331. Support for Advanced Component Research

FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687
SNL Contact: J. Borders, (505) 844-8855

We are applying various analytical instruments to the characterization of materials associated with the development of advanced components centered elsewhere in the laboratory.

Keywords: Analytical Instruments

Metallurgy Department, 1830

Department 1830 selects, develops, and characterizes the non-electronic behavior of all metals and processes that may be needed to meet systems and components requirements. Responsibilities span exploratory development through design, production, and stockpile life. If either current or anticipated demands cannot be met by commercially-available metals and processes, Department 1830 is responsible for the necessary development. Understanding mechanisms of alloy bulk and surface behavior provides the basis for alloy and process development and increases the confidence of predictions of behavior. Surface treatment and coating processes receive special emphasis because of the close coupling of the surface and "bulk" behavior.

Physical and Joining Metallurgy Division, 1831

The Physical and Joining Metallurgy Division selects, develops and characterizes the physical behavior of all metals that may be needed to meet systems and components requirements. This includes the selection and development of alloys to insure a sufficiently long service life while maintaining fabricability. Responsibilities span exploratory development through design, production and stockpile life. If commercial technology does not meet engineering requirements, Division 1831, working with the other divisions in Department 1830, will develop the required technology. Understanding the relationship between alloy processing, alloy microstructure and alloy behavior is the basis for alloy selection and development and provides the input required to predict, via thermodynamic and kinetic modeling, the physical behavior of the alloy through its service life. The objective of Division 1831 is, therefore, to use this understanding to extend the capabilities of the design engineers and to increase confidence in alloy performance.

Materials Properties, Behavior, Characterization or Testing

332. Weldability of Alloys — FY 1990 $125,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: C. V. Robino, (505) 844-6557, M. C. Maguire, (505) 844-1625, G. A. Knorovsky, (505) 844-1129, and M. J. Cieslak, (505) 845-9144

The response of alloys to welding operations is an important consideration in the recommendation of the material for component designs. Advanced materials, such as new investment cast martensitic stainless steels, aluminum alloy metal-matrix composites, nitrogen-strengthened wear-resistant stainless steels, and multi-layer clad alloys are being studied to determine optimum process control parameters for welding. These materials, as prototypes for many similar alloys, will help provide a more fundamental understanding of how welding defects, such as hot cracks, occur during production.

Keywords: Solder

333. Segregation Behavior During Solidification of Alloys FY 1990 $50,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: C. V. Robino, (505) 844-6557 and M. J. Cieslak, (505) 846-7500

Alloying element segregation is an important consequence in the solidification of welds in many engineering materials. Under certain conditions, selected elements may form minor low melting point constituents which remain in the last liquid to solidify. Under the stresses generated during cooling, the material may crack (called hot-cracking) in the region containing these low melting point constituents. To understand this behavior, the distribution of elements following solidification must be known quantitatively. The current program is solving the solidification problem more rigorously than has been done in the past. Diffusion in the solid, solidification in multicomponent systems and non-planar front solidification are being treated.

Keywords: Welding

334. Solid State Reactions Between Metal Substrates and Solders FY 1990 $100,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: P. T. Vianco, (505) 844-2329 and A. D. Romig, (505) 844-8358

Reactions between fusible alloy solders, based on Pb, Sn, In, etc., and metallic substrates such as Au and Cu can occur at room temperature. The most common manifestation of these reactions is the formation of intermetallic compounds. These compounds alter the mechanical and electrical performance of the solder joint, often degrading performance and reliability. In an integrated experimental and diffusion modeling program, a variety of important systems are being examined. The experimental efforts are aimed at determining the stability of the intermediate phases as a function of temperature and at determining the stability of the intermediate phases as a function of temperature and at determining the rates at which they form. Both bulk alloy and thin film substrates are under study. The modeling efforts are directed at determining reaction constants and activation energies and at using the results to model joint behavior through a variety of potential thermal cycles. Systems currently under study include Au/Pb-In, Au-Pd/Pb-In, Cu/Pb-Sn, Cu/Pb-In, and Pd/Pb-In.

Keywords: Solder

335. Fluxless Soldering FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: F. M. Hosking, (505) 844-4925

Fluxes promote wetting when soldering, but present potential long-term reliability problems with respect to the potential for corrosion if their residues are not removed. Reducing gases, such as molecular hydrogen or formic acid, are sometimes used to circumvent fluxing. Thermodynamic modeling suggests that atomic and/or ionic hydrogen should be more effective. In this study, the feasibility of using nonmolecular hydrogen and other atmospheres to reduce surface oxides and enhance wetting is being examined. The goal of this work is to find a reactive gas and specific processing conditions which produce solder joints which are comparable to those produced using rosin based fluxes, but are not environmentally hazardous either alone or with subsequent cleaning operations.

Keywords: Solder

336. Weld Process Development FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: P. W. Fuerschbach, (505) 845-8877, G. A. Knorovsky, (505) 844-1129, C. V. Robino, (505) 844-6557, and M. C. Maguire, (505) 844-1625

The use of welding processes in the manufacture of sophisticated, high technology hardware requires an understanding of the controlling mechanisms by which they operate. Optimization of the process is then possible. Heat input minimization to maximize melting efficiency in gas-tungsten-arc and plasma-arc welding has been quantified and a functional relationship developed which guides optimization of melting for a given material, process, and weld joint design. The mechanical response of resistance weld heads has been characterized and its influence on weld processing is being evaluated. Fundamental studies of variable polarity plasma arc welding and ultrasonic welding continues. A method of *in situ*, non-destructive evaluation of penetration in laser welding is being developed.

Keywords: Welding, Joining

Packaging and Structural Metallurgy Division, 1832

The mission of the Packaging and Structural Metallurgy Division 1832 is to provide the understanding and characterization of the mechanical, friction, and wear properties of materials. 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 Preparation, Synthesis, Deposition, Growth or Forming

337. Solid Film Lubrication Studies

FY 1990
$60,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: M. T. Dugger, (505) 844-1091

Solid film lubricants are under development for use in very clean environments. These films must adhere well to the substrate and generate only small amounts of debris in the wear process. Available films are being characterized and novel methods of $MoS_2$ deposition will be examined in terms of both productivity and performance.

Keywords: Friction, Wear, Lubrication

Materials Properties, Behavior, Characterization or Testing

338. Wear Modeling of Ceramics

FY 1990
$77,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: M. T. Dugger, (505) 844-1091 and R. J. Bourcier, (505) 844-6638

Develop a model to simulate the wear of ceramic surfaces using fundamental materials properties and the statistical parameters that characterize the surface topography on an appropriate microscopic scale. Measure topographical characteristics of actual wear surfaces using atmoic force microscopy and use these data to refine and validate the modeling.

Keywords: Friction, Wear, Ceramics, Modeling

339. Wetting and Mechanical Behavior of Interfacial Intermetallic in Solder Joints

FY 1990
$52,00

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: D. R. Frear, (505) 845-9023 and J. J. Stephens, (505) 845-9209

Intermetallics play an important role in the formation and mechanical response of solder joints. This program examines the wetting, the growth kinetics, and the resultant mechanical response of several intermetallics of interest in solder applications.

Keywords: Intermetallics, Solder, Fracture

340. Stress Corrosion Cracking - Modelling 2-D Crack Growth | FY 1990
$77,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: R. J. Bourcier, (505) 844-6638 and W. B. Jones, (505) 845-8301

The observed behavior of actual stress corrosion cracks growing through an alloy often times has an apparently probabilistic characteristic. Microscopic models exist to explain the one dimensional growth of stress corrosion cracks, but these provide no inherent insight into the two dimensional cracking characteristics. A two dimensional model is being developed to enable us to predict the actual crack growth which occurs in stress corrosion cracking specimens. Features such as microstructure and applied stress field are incorporated into the model.

Keywords: Corrosion, Stress Corrosion, Modeling

341. Al-Cu Thin Film Studies | FY 1990
$37,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contacts: D. R. Frear, (505) 845-9023 and A. D. Romig, (505) 844-8358

Al-Cu metallizations on integrated circuits are known to be more electromigration resistant than pure Al films. There is also evidence that the Al-Cu alloy also resists stress voiding better than pure Al. The mechanisms responsible for this behavior is not understood, although numerous hypotheses have been put forth, none has been validated. The microstructure of Al-Cu films will be varied through deposition conditions and thermal treatments. Analytical electron microscopy will be used to examine the distribution of Cu within the microstructure and the changes in distribution which result from electromigration testing to determine the mechanisms producing enhanced performance.

Keywords: Precipitation, Thin Films, Electromigration

342. Stress Voiding in Aluminum Metallizations | FY 1990
$200,000

DOE Contact C. B. Hilland, (301) 353-3687
Sandia Contacts: J. A. Van Den Avyle, (505) 845-8034, R. J. Bourcier, (505) 844-6638, and F. G. Yost, (505) 844-5446

The measurement and prediction of stresses in passivated aluminum metallization conductor lines on integrated circuits is key to the prediction of stress voiding. Experimental and analytic studies are underway to measure these stresses by X-ray diffraction and to model them using finite element methods. The results of this study will be used in developing and validating microstructurally-based models for the stress voiding process.

Keywords: Integrated Circuits, Voiding, Modeling

Melting Research and Solder Processing Division, 1833

This Division supports the laboratories by selecting, characterizing, and developing metallurgical processes needed in the manufacture of components and systems. The objective is to provide process definition and control by understanding the mechanisms which operate. Principal processes currently under study include laser welding, vacuum arc remelting, electroslag remelting, electron beam melting, investment casting, plasma spraying, and fluxless soldering.

Materials Preparation, Synthesis, Deposition, Growth or Forming

343. Investment Casting

FY 1990
$80,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: F. J. Zanner, (505) 844-7073

Investment casting is being studied with the objective of understanding fluidity as a function of alloy, mold material, mold temperature, and pouring temperature. Fluidity is an important physical parameter needed in modeling of the process in the support of computer integrated manufacturing.

Keywords: Fast Cast, Rapid Prototyping, Efficient Designs

344. Plasma Spraying

FY 1990
$120,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: M. F. Smith, (505) 846-4270

Atmospheric and low pressure plasma spray processes are being developed to produce coatings with desirable tribological properties. Process development is supported by a physical model of the process that has been developed that provides accurate predictions of plasma velocities and particle temperatures. Development of plasma sprayed diamond coatings has been initiated.

Keywords: Coatings, Plasma Spray

Device or Component Fabrication, Behavior or Testing

345. Laser Welding

FY 1990
$80,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: J. L. Jellison, (505) 844-6397

Both pulsed and CW laser welding is being developed for application to component closures. An 1800 watt CW Nd:YAG laser has been developed. Quantitative measurements of fluid flows are being made to support continued development of the physical model of the process.

Keywords: Beam-Material Interaction, Calorimetry

Corrosion, Cleaning and Thin Film Technology Division, 1834

The Corrosion, Cleaning and Thin Film Technology Division 1834 conducts applied research in the areas of atmospheric, aqueous and stress corrosion. The division elucidates corrosion mechanisms using electrochemical impedance spectroscopy and acoustic sensing devices. Cleaning and contamination control processes are developed. The efficacy of these processes is studied using electron spectroscopies (AES and XPS). Thin film deposition processes are developed as a way to achieve desirable surface properties (wear resistance, corrosion resistance, electrical conductance or insulation, lubrication, etc.). Electrochemical and physical vapor deposition techniques are stressed.

Materials Preparation, Synthesis, Deposition, Growth or Forming

346. Development of Multilayer Metallizations

FY 1990
$63,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: Dale C. McIntyre, (505) 844-2360

A facility has been constructed that allows multilayer metallizations to be designed using PVD techniques. This can be done with or without the addition of reactive gases or ion bombardment. These film structures are primarily designed for sealing non-metallic and metallic objects.

Keywords: Optical Fiber Metallization, Optical Fiber Hermetic Packaging

Materials Properties, Behavior, Characterization or Testing

347. Corrosion of Aluminum Metallization on Microelectronics FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: Diane E. Peebles, (505) 845-8087

Corrosion of aluminum metallization on VLSI is being studied as a function of Cu and Si content, fluoride ion contamination (due to HF etching processes), and metal deposition parameters. AES and XPS, as well as electrochemical impedance spectroscopy, are being used to elucidate the corrosion mechanisms/kinetics.

Keywords: Corrosion, Aluminum, Copper, Oxidation

348. Characterization of Diamond Films for Tribological Applications FY 1990
$83,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: Diane E. Peebles, (505) 845-8087

Diamond films are being deposited for tribological applications using several techniques (CVD, PVD, and plasma spray). Non-destructive techniques for characterizing these films using electron and optical spectroscopies have been developed. Film degradation in reactive atmospheres is being studied. The tribological properties of these films, as well as their adhesion to selected substrates, are being examined.

Keywords: Diamond, Diamond-like Carbon, Characterization

Device or Component Fabrication, Behavior or Testing

349. Development of Fiber-Optic Metallization for Joining FY 1990
$58,000

DOE Contact: C. B. Hilland, (301) 353-3687
Sandia Contact: Dale C. McIntyre, (505) 844-2360

Multilayer metallizations are being developed as graded seals for soldering fiber optics into metallic headers. Physical vapor deposition techniques are being developed to reduce the stress in the metallizations on very small diameter glass fibers. Barrier layers are being designed to diminish long-term reliability problems arising from intermetallic compound formation during and subsequent to the soldering process.

Keywords: Optical-Fiber Metallization, Optical Fiber Hermetic Packaging

Chemistry and Ceramics Department, 1840

Department 1840 supports Sandia weapons and energy programs by selecting, developing, and characterizing ceramics, glasses and glass-ceramics. A variety of approaches are used, including gas-phase synthesis and reactions, solution preparation, as well as more traditional ceramic processing. The department promotes advanced weapons and energy concepts by providing new materials and developing new prototype components.

Interfacial Chemistry and Coating Research Division, 1841

Division 1841 is responsible for developing an understanding of the materials and processes involved in the formation of coatings and thin film structures. This work may be applicable to processes in use at Sandia, such as CVD tungsten films, as well as to new types of coatings, such as electrophoretic formation of dielectric films. The division develops CVD and aerosol techniques for preparing ceramic powders. There is a major effort in understanding the interaction of hydrogen with metals.

Electronic Ceramic Division, 1842

Division 1842 develops and determines the properties of new ceramics for electronic and optical applications in Sandia systems. Examples are PZT for nonvolatile, radiation hard semiconductor memories, high-field ZnO varistors, $KNbO_3$ for optical switches, and cuprate high temperature superconductors.

Ceramics Development Division, 1845

Division 1845 is responsible for supporting laboratory programs involving glass- or ceramic-to-metal seals and other uses of glass or ceramics in moderate temperature environments. Expertise in the division includes the following areas: fracture surface analysis of brittle materials; seal design and fabrication processes; and glass and ceramic properties, i.e., strength, electrical conductivity. The division also maintains an active materials development program to formulate new glass or glass ceramics to meet particular requirements, e.g., corrosion resistance or high thermal expansion.

Inorganic Materials Chemistry Division, 1846

Division 1846 develops new processes for making ceramic powders and films using solution chemistry techniques. Understanding the structure and chemistry of sol-gel bulk and film materials is a significant part of this activity. The division also develops understanding of small particle-metal interactions that has led to new catalyst materials.

Materials Preparation, Synthesis, Deposition, Growth or Forming

350. Electrolytic and Electrophoretic Methods for Materials Processing FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Alan Hurd, (505) 846-6753

Electrophoresis as a technique has been used for some time to apply organic and ceramic coatings to large, irregularly-shaped objects. Our research has been directed towards the application of electrophoretically-deposited organic and organic/ceramic composite coatings as insulators and IEMP hardeners for electronic component packages. Present systems under study include acrylic/fluorocarbon copolymers and acrylic/titanium dioxide composites. New work includes the development of insulator/conductor composites.

Keywords: Coatings and Films, Polymeric Insulators/Dielectrics, Ceramic Insulators/Dielectrics, Electrophoretic Deposition

351. Aerosol Production of Fine Ceramic Powders FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Alan Hurd, (505) 846-6753

We are developing a generic method to coat powders. The objective is to coat some powder, A, with B, such that subsequent processing may be assessed for its compatibility with B. The nature of A then becomes irrelevant and may be changed at will with no effect on the process. We use an aerosol method since particle agglomeration is minimized. The powder ($<1\mu m$ in diameter) is entrained in a carrier gas and the coating material condensed on it and reacted further if necessary. We are currently characterizing the instrumentation (atomizer, condensation nuclei counter) and have begun to use it to atomize and measure prototype aerosols.

We have coated 38-75 $\mu m$ titanium powder in a fluidized bed at deposition conditions of 50 torr and 325°C using 30 percent diborane in argon. Powders with Ti:B ratios ranging from 2.9 to 0.5 ($TiB_2$) have been made. There was some concern that these powders would not press due to the hard boron coating. Although a free-standing pellet may not be possible, the powders were successfully pressed into a cup-like fixture, which is sufficient for some devices.

Keywords: Aerosols, Ceramic Powder, Coatings

352. Chemically Prepared Ceramic Films for Opto-Electronic Applications

FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: B. C. Bunker, (505) 844-8940

Most of the attention in the processing of ferroelectric thin films in the PLZT ((Pb, La)(Zr, Ti)$O_3$) family has focused on the preparation of PZT and PLZT. We have recently fabricated PLT thin films which are also of considerable interest to Sandia for a variety of applications. PLT materials offer a number of unique properties compared to PZT and PLZT. First, PLT materials have very high pyroelectric coefficients, making them an excellent choice in pyroelectric detector applications. Second, PLT films with large lanthanum contents have very high second order electrooptic coefficients and thus, films of those compositions are suitable for a number of optical applications.

Still other unique properties of PLT make it an interesting alternative material to PZT for non-volatile memory applications. PLT displays less of a tendency than PZT to form a detrimental pyrochlore phase during crystallization, and therefore, the perovskite phase forms at a lower temperature. This should result in improved compatibility with existing semiconductor processing technology. Also, PLT thin films (with higher lanthanum concentrations) prepared by rf-sputtering have displayed reasonably low coercive fields, making them suitable for use in non-volatile memory applications.

We have prepared high quality ferroelectric PLT thin films with lanthanum concentrations varying from O (pure $PbTiO_3$) to 25 mol% (i.e., PLT 25/100) by a chemical solution deposition method. The method we have developed uses hexane-based solutions of carboxylate, $\beta$-diketonate and alkoxide precursors, and allows for incorporation of large amounts of lanthanum (up to 25 mol%). Solution deposition processing of these materials is of interest because it is relatively inexpensive, rapid, and comparable with standard semiconductor processing technology.

We studied both the crystalline behavior of the films and the effects of composition (lanthanum doping level) on the dielectric and ferroelectric properties. As predicted, crystallization to the perovskite structure occurred at the relatively low temperature of 450°C, about 100°C lower than the crystallization temperature for PZT thin films. The dielectric constants of the films increased with increasing lanthanum doping from ~80 to ~690 for La contents varying from 0 to 25 mol%. The values obtained for the dielectric constants were in good agreement with those of PLT thin films prepared by rf-sputtering, although they were somewhat lower than those obtained for bulk PLT ceramics. The observed variation in the cure temperature with lanthanum concentration too verified the incorporation of lanthanum into the perovskite crystal structure.

We also characterized the ferroelectric properties of the films and found that, in general, the ferroelectric hysteresis loops became narrower and more symmetric with increasing lanthanum content. Coercive field decreased with increasing La content, as observed previously for rf-sputter deposited films. For a lanthanum content of 20 mol%, a coercive field of 19.8 kV/cm was obtained. This is approximately two-thirds the value of the coercive field typically obtained for solution derived PZT thin films. Remanent polarizations ranged from 12.9 to 1.8 $\mu C/cm^2$ for lanthanum concentrations varying from 5 to 20 mol%. Although these values are still sufficiently large for use in a non-volatile memory, they are somewhat lower than those reported for the rf-sputtered films. Reasons for this discrepancy are under study.

Keywords: Ceramic Coatings, Chemical Synthesis, Ceramics

353. Development of New Glasses and Glass-Ceramics | FY 1990
$250,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Peter Green, (505) 845-8929

We have developed a new family of $Fe_2O_3$-doped alkali aluminophosphate glasses (the NAFP-series) that have the bulk properties necessary to make durable seals to high expansion metals such a some Al-alloys and the 300 series stainless steels. Glass compositions exist with thermal expansion coefficients that match Al-4043 ($\approx 195 \times 10^{-7}/{}^\circ C$) and the aqueous durabilities comparable to silicate sealing glasses ($\approx 10^{-9}$ $g/cm^2$-min weight loss rate in 70°C water), two orders of magnitude better than CON-2. We have made hermetic, crack-free seals with Al-4043 (and 304 stainless steel) pins and Al-6061 shells. The glasses also strongly bond to Al-5456.

We have developed a group of lithium silicate glass ceramics that are being used to make hermetic seals to a variety of stainless and superalloys for actuator headers and other electronic components. A family of phosphate-based glasses is being used to form seals to Al, Cu, and stainless steels. Previously we developed a new glass that is very corrosion resistant to Li ambient temperature battery environments. This glass is presently used in batteries (active and reserve) and has an expected life of five years. We have developed a more advanced sealing glass with a 10-year life and have begun using it to replace the earlier, shorter-lived version. Transformation-toughened glass ceramics based on the precipitation of metastable $ZrO_2$ in a glass matrix have been developed. The objective of this program is to develop tougher glass ceramics for electrical insulator applications.

Keywords: Ceramics, Glasses, Electrical Insulators, Corrosion

354. Preparation of Ceramic Powders by Chemical Techniques | FY 1990 | $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: D. H. Doughty, (505) 844-1933

High-purity, homogeneous ceramic powders are being prepared by sol-gel chemistry techniques. Materials prepared include $ZrO_2$, PZT, ZnO, $Al_2O_3$, and titanate catalyst supports. The first three materials are utilized in ceramic electronic components at Sandia. Alumina is being toughened by coprecipitation with $ZrO_2$. The catalysts are used in our coal liquefaction program currently, and may find more general application. Novel glasses are also being prepared by sol-gel techniques. Our studies include basic research on precursors as well as applied development. Experimental techniques include small angle X-ray scattering, nuclear magnetic resonance, and several spectroscopic techniques to characterize precursor solutions and products. Glasses have been successfully evaluated on solar thermal receiver tubes and on photovoltaic cells. Dielectric barriers for a number of weapon applications have also been developed and are being evaluated.

Keywords: Ceramics, Glasses, Chemistry, Surface Characterization and Treatment

## Materials Structure and Composition

355. Structure of Novel Glasses | FY 1990 | $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Peter Green, (505) 845-8929

The goal of this program is to develop a general understanding of the relationships between the structure and properties of a glass in order to design compositions for specific applications. To that end, we characterize the effects of composition on the structures of simple glasses, using a number of spectroscopic techniques including X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and magic angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy.

We have characterized the short-range structures of at least 20 Sn-P-O-F glasses, prepared both at SNL and the University of Missouri-Rolla, using X-ray photoelectron and Raman spectroscopies. We have found that F plays a significantly different structural role than is reported in the literature. In glasses in which the P/Sn ratio is greater than the pyrophosphate composition, F is primarily bonded to P, whereas in glasses with lower P/Sn ratios, F-Sn bonds become significant. The elimination of P-F and P-O-P bonds appears to improve the resistance of the glass to chemical attack. This might explain why PbO additions significantly improve the glass durability; Pb-F bonds form at the expense of P-F bonds when PbO is added to a Sn-P-O-F base composition. One such glass, with 16 mole% PbO, has an aqueous durability comparable to CON-2, while retaining a significantly higher thermal expansion coefficient (~270vs. ~180x $10^{-7}/°C$) and much lower $T_g$ (115°C vs. 345°C). A hermetic Al-Al pin-seal was made with one of these glasses, although the glass-metal interface was crystallized and the glass became phase-separated.

Durable high expansion (>250 x $10^{-7}/°C$), low temperature ($T_g$ <150°C) glasses can be made based on the $P_2O_5$-$SnF_2$-SnO system. These glasses have been used to make optical components by low-temperature molding operations and as host materials to encapsulate organic molecules with interesting nonlinear properties. In addition, compositions with outstanding durability may also prove useful for high expansion sealing applications. Little is known, however, about the structure of these novel glasses and so it is difficult to design compositions for specific applications.

Keywords: Ceramics, Glasses, Electric Insulators

356. Structure of Sol-Gel Films | FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: D. H. Doughty, (505) 844-1933

Control of the microstructures of sol-gel-derived thin films (e.g., pore volume, surface area, pore size, refractive index) is important for such applications as protective and planarization layers, dielectric passivation layers, and sensor surfaces. This collaborative program explores the fundamentals of sol-gel film deposition using such techniques as imaging and conventional ellipsometry, FTIR microscopy, and gas sorption on SAW substrates.

During sol-gel thin film formation, inorganic precursors are assembled on the substrate surface by gravitational or centrifugal draining accompanied by vigorous solvent evaporation and further condensation reactions. Ellipsometric imaging of mixed water-alcohol solvents shows that water may be concentrated at the drying line. Therefore film deposition from coating sols containing water in excess of the azeotropic composition may occur primarily within water rather than alcohol. Based on surface area analyses of bulk gels, we found that replacement of alcohol with water causes a dramatic compaction of the structure in the final stage of drying. No doubt a similar effect occurs in thin films, which may explain the observation that film refractive indices increases with the $H_2O/M$ ratio of the precursor sol.

Finite element analyses of dip-coating alcohol-water mixtures showed a local maximum in $\gamma$ near the reservoir surface (275 $sec^{-1}$) and a maximum value of ~1000$sec^{-1}$ near the drying line. Since one model of the concentration dependence of viscosity predicts $\eta \sim \eta_o (1-\chi)^4$ where $\chi$ is the volume fraction of solvent, we believe that the concurrence of high $\gamma$ and high $\eta$ near the drying line causes Pe to exceed one there, leading to the observed ordering. If ordering can be conferred to space filling polyhedral particles, it might establish a route to the preparation of thick film samples that do not crack during drying or sintering.

Keywords: Ceramic Coatings, Glasses, Sol-Gel, Films

Materials Properties, Behavior, Characterization or Testing

357. Molecular Beam Studies of Hydrogen in Metals — FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Sylvia Tsao, (505) 846-6753

The recombinative desorption of hydrogen on a metal surface is perhaps the simplest of all heterogeneous chemical reactions. However, at present, the details of the kinetics associated with this reaction are not fully understood. The most common technique employed for the study of desorption kinetics is Temperature Programmed Desorption (TPD). However, for exothermic occluders, such as Pd, the kinetics may be further complicated by absorption into the bulk, and the determination of surface kinetic parameters from TPD data is highly questionable. One approach to circumvent this problem is to monitor desorption kinetics under stand-state conditions. In this way, the net particle flux across any interface (gas-surface, surface-bulk) is identically zero, and hence, the surface kinetics are clearly decoupled from sub-surface processes. Molecular beams are ideally suited for steady-state kinetic studies since they are able to supply a constant, well-collimated flux of reactants to the surfaces over a wide range of crystal temperatures. Using molecular beam techniques, we have studied H/D steady-state isotope exchange on Pd.

For surface coverages below 0.4 monolayers, the activation energy, $E_a$, and pre-exponential factor, ν, are constant and have values of 18 kcal/mole and $10^{12}$ $sec^{-1}$ ($\sim 10^{-3}$ $cm^2$-$sec^{-1}$), respectively. At higher coverages $E_a$ exhibits repulsive behavior and rapidly falls to a full coverage limit of approximately 2 kcal/mole. Commensurate with the decrease in $E_a$ the pre-exponential factor shows compensatory decreasing behavior. The extracted coverage-dependent kinetic parameters reproduce the experimental waveforms exactly. In addition, the steady-state measurements, coverage-dependent kinetic parameters are extracted from analysis of conventional TPD spectra. While the TPD-derived kinetic parameters reproduce the experimental TPD spectra, they are in quantitative disagreement with the stead-state measurements. Specifically, the steady-state determined kinetic parameters yield recombination rates that are much greater (~1000x) than those obtained by analysis of the TPD spectra. These findings clearly indicate that the TPD spectra are severely perturbed by bulk absorption and that the surface kinetic parameters derived from them are incorrect. Using our steady-state derived kinetic parameters to re-analyze the experimental TPD spectra, we can ambiguously determine the partitioning between surface and bulk hydrogen during desorption. We find that the ratio of surface to bulk hydrogen decreases from a value of 0.5

to 0.03 over the temperature range (250K-450K) spanning the TPD desorption spectrum. The low temperature value of 0.5 is particularly intriguing and strongly suggests the existence of a sub-surface binding site that is nearly isoenergetic with the surface chemisorption well. Our current efforts are focussed on using the steady-state technique to determine the kinetics of CO poisoning of the H/D exchange reaction.

Keywords: Hydrogen Effects, Surface Characterization and Treatment, Surface Modification

358. Electronic Ceramics

FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
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Studies of electronic ceramics include: (1) development of high field ZnO-based varistors and understanding microstructure-property relationships; (2) development of ZnO and dielectric granules for lightning arrestor connectors; (3) studying the electrical transport properties of boron carbides for thermoelectric generator and neutron detector applications; (4) study of the electrical properties of PZT films for nonvolatile semiconductor memories; and (5) relating processing, microstructure and Jc in $YBa_2Cu_3O_{7-x}$.

Keywords: Ceramics, Ceramic Coatings, Electronic Structure

359. Ceramic Fracture

FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Peter Green, (505) 845-8929

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. For example, reliable mechanical performance of ceramic ferrites is critical to their use in a variety of weapons components. In our previous characterization of the fracture behavior of these materials, we observed that, in subcritical crack growth, the mode of fracture varies from primarily transgranular to primarily intergranular as the stress intensity factor, K, is increased from 0.7 to 1.5 $MPa{\bullet}m^{1/2}$. During intergranular fracture, crack-interface bridges are generated which suppress the K at the crack tip. The dependence of the amount of intergranular fracture on the value of K means that the concentration of bridges in the wake of the crack will depend on the K value during growth of the crack.

Although crack-interface bridging is recognized as the major contributor to the toughness of alumina and other ceramics that do not contain phases which transform under stress, the mechanism by which bridges suppress K is not understood. The ability to control the bridge concentration in ferrites by varying K offers an opportunity for some critical experiments to generate that understanding. The current experiment used that feature of ferrite fracture to test the predictions of Bennison and Lawn (J. Mater, Sci. 24 3169 (1989)). In particular, we wanted to examine the R-curve behavior of ceramics with cracks that are initially formed and propagated with bridges and compare that behavior with cracks which initiate without bridge formation but are subsequently propagated with bridge formation. We introduced cracks with bridges by indenting flexure bars in a dry environment (high K) and cracks without bridges by indenting under water (low K). Subsequent strength testing of the bars gave very good agreement to the predicted behavior.

Keywords: Ceramics, Glasses, Fracture, Strength, Corrosion

360. <u>Reactivity and Bonding of Glasses and Ceramics to Metals</u> <u>FY 1990</u> $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Peter Green, (505) 845-8929

We study reactions between metals and glasses or ceramics using sessile drop experiments and detailed analyses of reaction zones by SEM, TEM, Electron microprobe, AES and XPS techniques. Systems under development include glass-ceramic to 304 stainless steel, glass to aluminum, and Ti-containing alloys on alumina, mullite, and zirconia toughened mullite. The objective of these studies is to develop sealing techniques that give strong, hermetic bonds with minimum mechanical stress.

Keywords: Glasses, Ceramics, Surface Microstructure, Metal-Ceramic, Surface Phases, Surface Characterization and Treatment

<u>Device or Component Fabrication, Behavior or Testing</u>

361. <u>Sensor Development</u> <u>FY 1990</u> $100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: Sylvia Tsao, (505) 846-6753

Accurate measurement of moisture levels is important in assessing long-term reliability in a variety of electrical and mechanical systems. The goals of this collaborative program are

(1) to develop porous silicon-based technology for producing integrated moisture sensors, where signal processing circuitry is located on-chip with the sensor, and (2) to develop a sensor for testing hermeticity in ceramic and plastic integrated circuit packages. We fabricate capacitive moisture sensors based on the use of oxidized porous silicon (OPS) as the sensing element. Porous silicon (PS), which can have specific surface areas as high as 400 $m^2g$, is formed by making silicon the anode in an electrochemical cell containing hydrofluoric acid. Porous microstructure depends largely on the dopant type and concentration in the silicon. Oxidation of PS at high temperatures in an oxygen or steam ambient forms OPS, which can be porous or fully dense depending on the original PS structure and the oxidation conditions. After oxidation, a porous gold metallization layer is deposited on the OPOS and aluminumm or titanium/gold is deposited on the back of the silicon wafer to form the electrical contacts. When water vapor contacts the sensor, it passes quickly through the gold and adsorbs on the pore walls, thereby changing the effective dielectric constant of the porous layer.

Keywords: Moisture Sensors, Oxides, Dielectric Films

362. SAW Development | FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: D. H. Doughty, (505) 844-1933

The detection of organic species in water is important in the analysis of waste water as well as in the monitoring of drinking water. Since some polymers absorb organic species much readily than they absorb water, they should be useful for detecting the presence of organic contaminants in an aqueous system. The sensitivity of acoustic plate mode (APM) devices, which can be effectively operated in contact with liquids, to mass changes in a polymer film contacting the device can be used as the sensing mechanism.

A preliminary investigation into this type of sensor was performed using a polystyrene coated APM device. A characterization of device response as a function of the concentration of both methylene chloride ($CH_2Cl_2$) and carbon tetrachloride ($CCl_4$) was obtained. The organic species caused a detectable response: frequency shifts of 25 and 615 ppm for $CH_2Cl_2$ (16 percent of saturation) and $CCl_4$ (23 percent of saturation), respectively. The response for $CH_2Cl_2$ was relatively linear with concentration up to over 60 percent of saturation. Larger responses should be observed for polymers with large absorption capabilities as well as for thicker polymers. Even though polymers are not highly selective, they do exhibit selectivity for types of organics and, therefore, an array of sensors of this type should be useful for obtaining information about the concentration of various types of organic species in water.

Keywords: Organic Detection, Acoustic Plate Mode, Organic Sensors

Sandia National Laboratories - Livermore

Materials Preparation, Synthesis, Deposition, Growth or Forming

363. Powder Metallurgy

FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: J. E. Smugeresky, (415) 294-2910

In addition to extensive powder handling and characterization capabilities including automated image analysis, facilities exist to produce rapidly solidified structures by inert atomization, melt spinning, and spark erosion. Emphasis is being placed on the effect of processing parameters on material characteristics. We are also developing methods to produce metal powders via chemical precipitation processes.

Metallurgical studies are being conducted on a variety of alloy systems. The relationship between strength, toughness, microstructure, and fracture modes of blended elemental PM titanium alloys is being studied to optimize HIP cycles and heat treatments for improved properties of near-net-shape processed components. The relationships between starting powder size and sintering parameters on the microstructure, permeation and filtration characteristics of porous stainless steel compacts is being established. The dynamic compaction of Al-Si alloys has produced fully dense compacts, retained metastable microstructures of the original powder, and has provided further insight into the mechanisms at inter-particle bonding. The effect of particle size distribution and morphology on the quality of compacts is also being established. The new rapid solidification processing facilities will also be utilized to produce powders for metal matrix composites.

Keywords: Alloys, Rapid Solidification, Metals, Shock Wave Compaction

364. Advanced Electrodeposition Studies

FY 1990
$300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: R. E. Stoltz, (415) 294-2162, H. R. Johnson, (415) 294-2822, W. D. Bonivert, (415) 294-2987

Engineering applications, electroanalytical development, and fundamental studies are being pursued in the areas of electrodeposition and electroforming. Electrodeposition of a variety of metals is being studied with a focus on the relationship between critical process variables and the mechanical properties of the deposit. The role surface active agents play in this process is being studied using an in situ real-time monitor for organic additives developed at SNLL. We are particularly focusing on the development of environmentally acceptable electroplating methods and procedures.

Keywords: Metals, Electrodeposition, Electroforming, Mechanical Properties, Chromium

365. Metal Forming FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: D. A. Hughes, (415) 294-2686

Fundamental understanding of inelastic deformation is being developed through crystal plasticity modeling and experimentation. Recent studies in this area relate to the properties of metals which have been altered by deformation-induced anisotropy. We have obtained a complete set of constitutive model constants for an engineering material, 304L stainless steel. Companion finite element analyses of metal forming operations, including a 304L stainless steel closed-die extrusion process, are in progress. Additional, physically-based, insight for designing constitutive relations is emerging from studies of the evolution of dislocation substructures in large-strain torsion experiments. Recent results provide new evidence that these structures evolve in a stable manner without localized shearing. This observation is in sharp contrast to previous investigations which have emphasized instabilities in the formation of dislocation microstructures.

Keywords: Metals: Ferrous and Non-Ferrous, Fracture, Near-Net-Shape Forming

366. Advanced Foam Materials FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: D. L. Lindner, (415) 294-3306 and W. R. Even, (415) 294-3217

Recent developments in our understanding of the relationship between microstructure and macroscopic properties in preparation of low density foam materials has led to the ability to produce foams with unique physical properties and tailored chemical properties. Engineering applications and basic studies designed to optimize properties are being pursued. We have begun determining the relationship between these unique microstructures and physical and mechanized properties of the foams. We have been successful in producing a continuum in morphologies ranging from very open cell-low density, to nearly closed cell-higher density polymeric foams. We have developed several different methods to produce such materials in a variety of modifications. These materials have demonstrated utility as catalyst support structures or low-pressure-drop, high-efficiency filters.

Keywords: Polymers, Catalysis, Molding, Microstructure

367. Tritium Getter Technology

FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: D. L. Lindner, (415) 294-3306 and T. Shepodd, (514) 294-2791

We are investigating the use of solid alkynes and alkenes as organic tritium getters. Currently we use several alkynes as hydrogen getters in controlled environments (ie., in the absence of oxygen and water). We have demonstrated that the use of these materials can be extended to applications in which a limited amount of oxygen and/or water is present as well as investigating their use to getter tritium without producing HTO or gaseous tritided species as hazardous by-products. Work with 1,4-bis (phenylethynyl) benzene has shown that when mixed with appropriate catalysis, it can quickly getter tritium (as it does hydrogen). Aging studies of the tritiated getter demonstrate that no gaseous tritided species are evolved over extended periods of time. We are now modifying these getter systems to provide materials that will provide enhanced stability and functionality in the radiolytic environment.

Keywords: Hydrogen Getters, Tritium

368. Plasma Processing

FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: W. L. Hsu, (415) 294-2379

Plasma processes are used to develop new and advanced material coatings. In particular, hard amorphous carbon films and diamond films have been deposited for applications as tritium permeation barriers, corrosion barriers, and sealants against moisture absorption. Film growth is achieved by using a plasma discharge to break down and enhance the reactivity of the fill gas, which is typically a mixture of hydrogen and methane. The research program emphasizes three areas of investigation: gas phase chemistry induced by the plasma, nucleation kinetics, and characterization of film properties. In situ diagnostics, such as mass spectroscopy with energy filter, optical emission spectroscopy, and Langmuir probes, are developed for studying the plasma-gas phase reactions. Laser Raman spectroscopy has been applied for in situ film growth studies. A variety of analytical techniques such as TEM, SEM, ERD, and RBS have been used to characterize the deposited film structures. The goal of the program is to create pin-hole-free amorphous carbon films and single-crystal diamond films with good adhesion to a variety of substrate materials.

Keywords: Plasma Processing, Carbon-Based Materials, Amorphous Films, Diamond

Materials Properties, Behavior, Characterization or Testing

369. Tritium and Decay Helium Effects on Crack Growth in Metals and Alloys

FY 1990
$500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: S. L. Robinson, (415) 294-2209, S. H. Goods, (415) 294-3274 and R. Moody, (415) 294-2622

The effects of tritium and decay helium on the mechanical properties and crack growth susceptibility of fcc alloys are presently being studied. These studies begin with tests in high pressure hydrogen gas and with tests on hydrogen precharged samples to determine the effects of applied stress, microstructure, and thermomechanical processing on hydrogen-induced failure. The fundamental effects of hydrogen (and tritium which is chemically similar) on the mechanisms that govern plastic flow and fracture are then defined with these results. Similar studies are underway in samples exposed to tritium, which decays to helium without inducing radiation damage, to determine the added effects of decay helium on failure properties. With preliminary results from these studies and theoretical analysis based on the Embedded Atom Method developed at Sandia, we are beginning to define the effects of helium on properties, crack growth susceptibility, and on the mechanisms of plastic flow and fracture.

Keywords: Metals: Ferrous and Non-Ferrous, Crystal Defects/Grain Boundaries, Fracture

370. Joining Science and Technology

FY 1990
$400,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: J. A. Brooks, (415) 294-2051, K. W. Mahin, (415) 294-3582, M. L. Callabressi, (415) 294-2064

We are directing considerable effort toward developing a science-based methodology for designing, analyzing, characterizing 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 temperature, residual stresses, and elemental segregation.

Additional welding metallurgy activities include the evaluation of alloy modifications to improve the weldability of specific alloys, the evolution of weld microstructure during solidification and cooling, the study of weldment cracking mechanisms, the weld microstructure property relationships, and analysis of joints in composite materials. In solid state welds, the current emphasis includes establishing specifications for weld evaluation and acceptance, and improved NDE techniques to verify weld quality. Alloy systems of current interest include austenitic and martensitic stainless steels (single phase and precipitation hardenable), titanium, and model alloy systems.

Keywords: Joining and Welding, NDE, Microstructure, Metals, Transformation, Solidification, Modeling

371. Composites: Characterization and Joining — FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: D. L. Lindner, (415) 294-3306 and J. R. Springarn, (415) 294-3307

The stability, compatibility, and joining of organic matrix composite materials are being investigated. The work focuses on graphite-fiber-reinforced composites and includes both thermosetting and thermoplastic matrix materials. Coatings for composite materials are under investigation to enhance stability for special design needs (e.g., mirrors). We are also developing coatings for the protection of composite materials in high temperature oxidizing environments.

Joining of composite materials is being studied and includes mechanical fasteners, adhesives and the welding of thermoplastics. Techniques are being developed to measure the fracture toughness of adhesive bonds and predict the strength of mechanically fastened joints.

Keywords: Composites, Joining and Welding, Fibers, Corrosion, Coatings

372. Compatibility, Corrosion, and Cleaning of Materials — FY 1990 $50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: R. E. Stoltz, (415) 294-2162, H. R. Johnson, (415) 294-2822 and D. K. Ottesen, (415) 294-3687 and J. M. Hruby, (415) 294-2596

Examination of surfaces to determine compatibility, corrosion, and cleanliness is being carried out using state-of-the-art electroanalytical and spectroscopic means. Many potential problems exist during production and assembly of components if parts are not properly cleaned. However, it is difficult to quantify cleanliness and many parts have interiors inaccessible for examination by conventional methods. We have developed a unique technique using Fourier transform infrared spectroscopy that is capable of peering inside small diameter tubes or examining small diameter wires to identify wall-surface contamination. This method has been shown to be robust in a production environment we are also developing, characterizing and qualifying for use a range of alternate cleaning methods for metals. The intent is to minimize use of hazardous materials and to reduce waste.

Keywords: Compatibility, Corrosion, Cleaning, FTIR

373. Helium in Metal Tritides — FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: W. A. Swansiger, FTS 234-2496, S. E. Guthrie, FTS 234-2360 and D. F. Cowgill, (505) 844-7480

The evolution of helium in metal tritides is being studied by NMR, gas volumetry and dilatometry techniques. NMR measurements carried out over the past year are a continuation of prior work on the determination of helium densities in bubbles of aged Pd through the observation of the solid, liquid, gas phase transitions of the helium trapped in the bubbles. Initial tests have been completed on a sensitive gas sampling system to measure in real time the evolution of helium from metal tritides. Changes in the phase behavior of Pd tritide as a function of He bubble content have been determined by gas volumetry and correlated to measurements of physical size changes due to the dilation of the metal lattice with the evolution of bubbles.

Keywords: Helium, Metal Tritides

## Instrumentation and Facilities

374. Tritium Facility Materials Characterization and Testing — FY 1990 $300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contacts: S. H. Goods, (415) 294-3274 and S. L. Robinson, (415) 294-2209

Exposure to tritium is now known to degrade the performance of many structural and containment materials. Materials research needs in the Tritium Research Laboratory have driven the acquisition of new analytical techniques and equipment and the upgrading of existing experimental test equipment. New capabilities being developed include, quantitative $^3$He mass spectrometry for characterizing helium concentrations resulting from tritium decay, and induction heating capability for rapid thermal cycling of small tritium charged metallic specimens. A new high-pressure $T_2$ thermal charging and quench facility is yielding precise measurement of tritium solubility as a function of pressure and temperature in a variety of materials. A new Auger spectrometry system allows us to analyze surface compositions.

Computerized data acquisition has been added to the servohydraulic mechanical test frame. Characterization of fracture phenomena is facilitated by a modern scanning electron microscope. These capabilities contribute to the characterization and prediction of tritium-induced degradation phenomena in containment materials.

Keywords: Spectrometer, Tritium Charging, Mechanical Testing, Scanning Electron Microscopy

375. <u>New Analytical Techniques</u>

FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: M. C. Nichols, (415) 294-2906

New spectroscopic and analytical techniques are being developed for special applications. For example, we have developed a system for chemically selective X-ray microtomography. We are employing this technique to image microstructure in a variety of materials, work this year has demonstrated that microscopic details in metal matrix composite materials can be imaged and that microcracks in materials under load in a specifically designed test frame can be examined.

Keywords: X-ray Tomography, Chemical Analysis

376. <u>New High Resolution Electron Microscopy Facility</u>

FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
SNL Contact: M. J. Mills, (415) 294-3018

A new high resolution transmission electron microscope laboratory is now operational. It includes an intermediate voltage high resolution microscope, sample preparation and photoprocessing facilities, and computational facilities for image simulations and image processing. It will be utilized to determine the atomistic structures of a number of material systems, including (a) metal-metal interfaces, such as grain boundaries, (b) defect structures in undeformed and deformed metals and alloys, (c) helium-induced defect evolution in metal tritides, and (d) semiconductor-oxide interfaces. These studies are important to gas transfer technologies and to semiconductor device fabrication.

Keywords: High Resolution Electron Microscopy, Interfaces, Grain Boundaries, Tritides, Semiconductors

Lawrence Livermore National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

377. Inorganic Aerogels

FY 1990
$350,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: L. W. Hrubesh, (415) 423-1691/FTS 543-1691

The approach is to perform a controlled hydrolysis of metal alkoxides such that the partially hydrolyzed chemical can be limited from further condensing reactions by using an appropriate buffer solvent. Subsequently, this pre-hydrolyzed chemical can either be diluted to make low density sol-gels, or directly gelled to achieve higher densities. Aerogels are obtained by super-critical solvent extraction of the wet gels.

We have successfully applied this approach to make silica aerogels starting with partially hydrolyzed tetramethoxysilane (TMOS). We have made transparent, monolithic silica aerogels with dimensions of 2.5 cm x 4.5 cm x 40 cm at selected densities over the range of 0.005 to 0.70 $g/cm^3$.

This material has unusual optical and thermal properties due to its ultrafine microstructure. Its applications include target material for direct drive laser fusion experiments, thermally insulating window glass, and as collector material for hyper-velocity microparticle capture.

Keywords: Inorganic Aerogels, Sol-Gel, Laser Fusion Targets

378. Photoactivated Catalysis on Aerogels

FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: C. A. Colemenares, (415) 422-6352/FTS 532-6352

A low density $SiO_2$ aerogel (50-100 $mg/cm^2$) doped with 0.45 wt% uranyl ions ($UO_{2++}$) was found to be photochemically active for the production of hydrocarbons from various gas sources. The energy source was a 1000-W Mercury-Xenox, solar-simulator lamp, which illuminated fine particles of aerogel suspended in a fluidized bed using the reaction-gas mixture. Experiments with a $2H_2$:1CO gas mixture produced mostly methane, ethylene, ethane, and propane. Products from a 1 $H_2$:1 $C_2H_4$ mixture were methane, ethane, propane, butane, pentane, hexane, and some unidentified products; while mostly ethylene with small amounts of methane were formed from a 1 $H_2$r:1 $C_2H_6$ gas mixture. Europium and cerium-doped $SiO_2$ aerogels have been prepared and we are in the process of evaluating them.

Basic studies of the energy transfer mechanisms have been initiated. We are using fast optical spectroscopic techniques, as well as ultraviolet and x-ray photoelectron spectroscopies to carry out these studies.

Keywords: Photoactivation, Silicon Dioxide

379. Organic Aerogels

FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: R. W. Pekala, (415) 422-0152/FTS 532-0152

Organic aerogels have been produced from the base catalyzed, aqueous reaction of resorcinol with formaldehyde. The aerogels have a microstructure composed of interconnected colloidal-like particles with diameters of 30-200 Å, cell sizes of less than 1000 Å, and surface areas of 400-900 $m^2/g$. This microstructure is retained even after carbonization at 1100°C.

Keywords: Organic Aerogels, Sol-Gel, Laser Fusion Targets

380. Polymer Materials Development and Coating

FY 1990
$1,000,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: S. A. Letts, (415) 423-2681/FTS 543-2681

New direct-drive laser fusion targets required development of new polymer materials and coatings. Microshells that incorporate iodine and other elements were fabricated for spectroscopic diagnosis of target performance. Preparation of microshells from the new polymers required better control and understanding of the shell-making process. The shells are overcoated by plasma polymerization. The plasma coating process was controlled to deposit materials of the desired composition. The new coatings required greatly expanded target characterization and materials analysis.

Keywords: Polymer Foams, Low-Density Materials, Laser Fusion Targets, Plasma Polymer Coatings

381. Atomic Engineering

FY 1990
$190,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: Troy W. Barbee, Jr., (415) 423-7796/FTS 543-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one dimension during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2 nm) to hundreds of monolayers (>100 nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 16,665 layers of each of two materials to form up to 63$\mu$m thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have strong potential for extremely high mechanical performance of metals as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing oils with strengths approaching those of whiskers.

Keywords: Thin Films, Multilayer Technology

Materials Structure and Composition

382. Theory of the Structure and Dynamics of Molecular Fluids — FY 1990 $300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: D. F. Calef, (415) 422-7797/FTS 532-7797

We have been developing and applying the methods of modern statistical mechanics to study the behavior of molecular fluids, especially under the high density and temperature conditions experienced by reacting explosive molecules. We are completing a computer code to calculate liquid mixture structures. The program calculates a complete set of thermodynamic properties using more realistic intermolecular potentials than any other currently available. The output of this program will also be used in calculating reaction "transition state volumes" and solvation dynamics. We are also developing molecular dynamic models for phase separations and carbon coagulation.

Keywords: Molecular Fluids, Prediction Behavior Modeling

383. Plutonium Pyrochemical Research — FY 1990 $25,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: H. Coops, (415) 423-4655/FTS 543-4655

The object of this effort is to demonstrate a practical technology to produce high purity plutonium metal from pure plutonium oxide by a process that does not generate intractable residues or chemical wastes. This would provide a replacement option for both the Bomb Reduction and Direct Oxide Reduction methods that generate large amounts of residues, with a process that operates on a closed chemical cycle, i.e., the reaction by-product can be electrochemically regenerated to form new reagent feed in a loop that can be recycled indefinitely.

The process is based on lithium-6 as the chemical reductant; the use of this isotope will eliminate ($\alpha$, $\eta$) neutron emission from plutonium reduction operations and will therefore decrease operator radiation exposure. We have demonstrated that ability of lithium to reduce $PuO_2$ in laboratory-scale experiments. The $Li_2O$ reaction produce can be reclaimed from the reaction mixture after isolating the produce metal by siphoning at 750°C. The excess lithium and the $Li_2O$ is recovered by distillation, and the $Li_2O$ regenerated (after chlorination) by electrolysis at 600°C, using known production technology (operational Y-12 process).

Keywords: Pyrochemical Processing

384. Electronic Structure in Superconducting Oxides | FY 1990 $1,290,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: M. J. Fluss, (415) 423-6665/FTS 543-6665

We have designated three experimental task areas: materials synthesis and properties, electron structure, and thin films, all of which are guided and supported by a broad theoretical task in band structure, ligand field effects, and pairing mechanisms. The selection of these activity areas provides the basis for a flexible, but focused program which is contributing to the solution of critical problems in the search for an understanding of the oxide superconductors. Additionally, the thrust is sensitive to opportunities for utilization of the new superconductors in future LLNL programs and has explored processing and applications oriented activities.

A variety of theoretical approaches have been used to study the nature of the charge carriers, the paring mechanism and the formation of a superconducting state in superconducting oxide materials. The properties of paired charge carriers of fractional charge in a superconducting mechanism were investigated as was the condensation of a two dimensional Bose-Coulomb gas. Calculations of the electronic structure of superconducting oxides were done based both on band theory and Hartree-Fock with configurational interactions. Both of these approaches suggested the importance of specific hole states in the superconducting mechanism. Results that directly describe laboratory experiments were obtained from the Hartree-Fock method for Mossbauer measurements and from linear combination of atomic and molecular orbitals in a cluster approach to describe electronic structure measurements made with positrons on several materials.

Keywords: Superconductors, Electronic Structure, Positron Annihilation

385. Electronic Structure of the Thermodynamic and Mechanical Properties of Al-Li Alloys

FY 1990
$180,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: A. Gonis, (415) 423-5836/FTS 543-5836

The first stage of this study consisted of calculating the equilibrium thermodynamic properties of Al-Li alloys across the concentration range, in both the fcc and bcc phases. Calculations of equilibrium charge densities, lattice constants, and energies of mixing have been completed for alloys based on both fcc and bcc crystal structures at selected concentrations. Calculations of effective pair interactions are underway. Our results indicate that the bcc-based alloys with lithium concentrations of 50 percent and 75 percent will order at low temperature in the B32 and $DO_3$ phases, respectively. This behavior is consistent with experimental and previous theoretical studies carried out on the basis of phenomenological models. Dilute Li alloys in the fcc phase, which are the technologically important ones, exhibit very rich behavior. The calculations of phase stability of fcc Al-Li alloys have also revealed a wealth of "unexpected" physical behavior.

Keywords: Electronic Structure, Grain Boundary, Surface

Materials Properties, Behavior, Characterization or Testing

386. Nuclear Spin Polarization

FY 1990
$1,100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: P. C. Souers, (415) 422-1301/FTS 532-1301

The triton polarization memory time has proved to be too short in regular solid D-T and 95 percent molecular DT absorption of the D-T on silica aerogel foam shows promise of lengthening the memory time. Design of an adsorption column to purify DT has begun. A Raman spectrometer intended to measure small $J=1$ $T_2$ levels in the DT is almost ready. Theory suggests that the deuteron should have a longer memory time and that triton-to-deuteron polarization may be possible. Electron spin resonance shows atom concentrations up to 1,000 ppm for use as pumpers in dynamic nuclear polarization. Heat spikes and a long electron relaxation time are negative findings. Design of a 0.5 K, 94 GHz polarization system, intended to be ready in 1992, has begun. This system will attempt polarization of the purified DT sample.

Keywords: Spin Polarization, Electron Spin Resonance

387. Measurement of Tritium Permeation Through Resistant Materials at Low Temperatures

FY 1990
$90,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: Jon L. Maienschein, (415) 423-1816/FTS 543-1816

We measure tritium permeation by capturing, in liquid, tritium that permeates through a sample membrane. The liquid is subsequently analyzed by liquid scintillation counting. Because our apparatus is simple and inexpensive, we can run many replicates of each material for the lengthy periods that are required to reach steady-state permeation behavior. We therefore get an accurate measurement of the permeation rate. The high sensitivity of liquid scintillation counting allows us to measure very low permeation rates. In prior tests with many polycrystalline metals, including aluminum, beryllium, cadmium, copper, gold, iridium, lead, molybdenum, rhenium, silver, and tungsten, we showed that tritium transport along defects dominates the permeation process. Therefore, permeation measurements at higher temperatures cannot be extrapolated to low temperatures. We have made permeation measurements on single crystal copper, and have shown that they are consistent with extrapolation of high temperature results in the literature. We are currently preparing specimens of single crystal beryllium. Our data on single crystal beryllium will be the only true measurement in tritium permeation through that material, as all other data in the literature were taken with polycrystalline samples where transport along defects dominates the permeation rate. Future work will include measurements on other single crystal metals.

Keywords: Permeation, Tritium, Liquid Scintillation Counting

388. Pretransformation Behavior in Alloys

FY 1990
$500,000

DOE Contact: A. Dragoo, (301) 353-5276/FTS 233-5276
LLNL Contact: L. E. Tanner, (415) 423-2653/FTS 543-2653

Our current research on diffusionless displacive phase transformations has shown that a parent lattice (i.e., the transforming phase) develops local atomic perturbations that are structurally related to the product phase (or phases) to be formed, and these perturbations are instrumental in the product phase nucleation process. It recently became apparent that such perturbations also play a crucial role in diffusional (or replacive) transformations. That is, there is a coupling between the displacive and replacive processes. To elucidate this behavior we are examining the thermal decomposition of the high-temperature-stable $Ni_xAl_{(100-x)}$ $\beta 2$ phase (cubic ordered B2, CsCl-type structure) with X - 62.5 and 65 to determine the sequence of transformations to the low-temperature phases: $Ni_2Al$ (metastable), 3R or 7R martensites (metastable), $Ni_5Al_3$ (stable) and $Ni_3Al$ (stable).

Keywords: Metals: Ferrous and Non-Ferrous, Predictive Behavior Modeling

389. The Structure Property Link in Sub-Nanometer Materials — FY 1990 $60,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: A. F. Jankowski, (415) 423-2519/FTS 543-2519

The structure-property link is critical in subnanometer scaled materials. This is especially true for microstructures with alternating layers composed of only a few atomic planes each—that is, multilayers with short wavelength composition modulations. Equilibrium atomic configurations and phase stability of metallic multilayer systems, such as Au/Ni, are investigated with high resolution electron microscopy and X-ray diffraction. The observed atomic structure is then linked with measured elastic and magnetic-optical behavior using the concept of strain relaxation from coherent interfaces.

Keywords: Films, Multilayers

390. Synchrotron Radiation-Based Materials Science — FY 1990 $800,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contacts: J. Wong, (415) 423-6385/FTS 543-6385

We have achieved a time resolution of 10 ms at the NSLS in a diffraction study of the Ni + Al reaction, which confirmed formation of intermediates with a focused beam and have successfully installed a second position-sensitive photodiode array detector to double the 20-space data acquisition in our TR-XRD measurements. New microstructural data for resorcinol-formaldehyde aerogels and for an aluminum multiphase alloy were obtained from SAXS and tomographic experiments, respectively. We constructed and demonstrated use of a load cell to perform *in situ* tomographic images under tensile loads to 100 kpsi. We also designed and successfully installed a new "quick-scanning" EXAFS (QEXAFS) capability at beamline 10-2 at the SSRL to perform time-resolved X-ray spectroscopic measurements on phase transformation and thin film deposition. Construction of a chamber for *in situ* thin film deposition with QEXAFS was completed.

Keywords: Synchrotron-Radiation, X-Ray Diffraction

391. Structural Transformation and Precursor Phenomena FY 1990
$150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: P. E. A. Turchi, (415) 422-9925/FTS 542-9925

Electronic property studies were performed with a realistic tight binding electronic Hamiltonian. The recursion technique was used to calculate densities of states and include A15, Laves phases (C14, C15 and C36), $Zr_4Al_3$ type of phase and sigma phase. We conclude that the strong interplay between geometrical factors and electronic parameters leads to a stability of these complex phases for an average number of d-electrons less than 6.0. The Fe-Cr system was selected as the first candidate to study precursor phenomena. Experiments at the Oak Ridge beamline X14 of the NSLS showed: (1) Fe-Cr is clearly a clustering system, as predicted by theory; the validity of the electronic parameters used gives us great confidence for future theoretical simulations of the bcc to sigma transformation; (2) maxima of intensity appear at the 2/3(111) positions, probably indicative of the intrinsic bcc-phonon softening seen in most of the bcc metals and alloys, and (3) the "topology" of the diffuse scattering changes with contrast, thus attributed to a strong displacement intensity. This encouraging result will make possible a detailed analysis of the local displacement field which could explain the structural transformation.

Keywords: Electronic Structure, Phase Stability

392. Underwater Explosive Energetics FY 1990
$150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. C. Tao, (415) 423-0499/FTS 543-0499

We have completed the development of an Ultrafast Microphotography Apparatus and a capacitor discharge ignition source for examining rapid combustion of metals in water. Using both streak and framing cameras, we have imaged the heatup of 28-76 microns diameter aluminum wires, the process leading to the fragmentation of the molten aluminum, and the subsequent rapid sustained reaction of the aluminum with water. By replacing the aluminum with a nonreactive metal, such as gold, and observing its thermal interaction with water, we have been able to separate the energy contribution to the vapor layer by direct heat transfer from that due to any exothermic chemical reaction. The current model can calculate the temperature of the aluminum as a function of the capacitor discharge voltage, predict the dimension of the vapor layer, and provide an estimation of the pressure distribution within the expanding bubble. Currently, the foci of the research are (1) improve the diagnostic techniques to measure the temperature of the wire after energy input and the pressure during the abrupt transition to raid sustained combustion (2) perform spectroscopic measurements to resolve the chemical kinetics of aluminum oxide formation, and (3) extend the model to include a full set of chemical reactions.

Keywords: Underwater Explosives, Reactive Metals

393. Composite Explosive Energetics

FY 1990
$150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. C. Tao, (415) 423-0499/FTS 543-0499

We have finished investigating the first series of bicomponent composite explosives, PETN/Al and TNT/Al, loaded with different weight percent of 5 micron spherical aluminum. The metal acceleration techniques chosen for this study prove to be quite versatile in detailing the reaction zone length for the reaction between the aluminum and the detonation products. In addition, we have been able to incorporate a calculational method, which involves reactive flow modelling and thermodynamic calculations with TIGER, to predict the extent of aluminum reaction within the early time expansion. We have planned additional PETN-Al experiments with longer charges and with flake aluminum rather than 5 $\mu$m spherical. It is our goal to understand the different physical, chemical, and thermal mechanisms influencing the complex kinetics associated with composite explosive systems in hope that we can tailor the rate of explosive energy delivery for various applications. We have addressed in this study experimental methods and approach to probing one of these mechanism; namely the role of metal additives and their rate and extent of reaction with a hot oxidizing medium. Concurrently, we are developing a reaction zone model, in contrast to a CI model, which will provide a realistic and useful description of the hydrodynamic response in composite explosives.

Keywords: Composite Explosives, Metal Loading, Reactive Flow Modeling

394. Low Vulnerability Explosives

FY 1990
$420,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: C. Pruneda, (415) 422-0460/FTS 532-0460

Previous low-vulnerability explosives (LOVEX) formulations were optimized to some extent with respect to performance, cost, and decreased vulnerability in 4-inch diameter hardware. However, these same formulations were not optimized with respect to, among other things, the binder cure chemistry, sympathetic detonation, and thermal stability (cook-off) in 8-inch diameter hardware. This report focuses on modification of the polymer binder and the formulation composition to improve both the quality of the cured explosive and the insensitivity of LOVEX formulations to sympathetic detonation in 8-inch diameter hardware. The thermal stability issue is the focus of ongoing work and will be addressed in future reports. We discuss the modified polymer system used and the 8-inch diameter sympathetic detonation test results of three LOVEX formulations RX-35-AQ, RX-35-AS, and RX-35-AT. LOVEX formulations have been developed which do not sympathetically detonate in 8-inch diameter hardware and which have very good low-viscosity processing properties.

Keywords: Insensitive Explosives

395. Fundamentals of Explosive Vulnerability — FY 1990, $400,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. C. Tao, (415) 423-0499/FTS 543-0499

The purpose of these studies is to establish correlations between the intensity of explosive response and the specific material characteristics of the explosive (i.e., the modulus, the energy of the binder, and the particle size of the energetic crystalline material).

In this program we are focusing on the effects of the physical properties of a main charge explosive that can be modified by formulation, and how that might be used to develop a more fundamental understanding of initiation. We are varying those properties that are expected to have the greatest affect on the sensitivity when a munition is exposed to multiple damage and initiation stimuli.

Keywords: Insensitive Explosives, Vulnerability

396. Very High Energy Density Materials — FY 1990, $50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: R. L. Simpson, (415) 423-0379/FTS 543-0379

An experimental effort was initiated with the epsilon form of CL-20 to examine its sensitivity and performance properties. An $\epsilon$-CL-20 analog to LX-14 was formulated. Data reported include: impact, spark, and friction sensitivities, differential scanning calorimetry and thermal gravimetric analyses, and one-dimensional-time-to-explosion (ODTX). Both the pure alpha and epsilon phases were examined as well as the epsilon based formulation. To examine questions concerning the effect of mechanical confinement on the ODTX results vented experiments were carried out. Performance measurements included a 24mm cylinder test, small scale metal acceleration experiments and particle velocity examination using impedance matched crystals.

Keywords: Explosives Characterization

397. Use of Finite Element Analysis to Understand Delayed Failure of Silver-Interlayer Welds

FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: G. A. Henshall, (415) 423-4655/FTS 543-4655

There is currently a growing interest in the use of thin (e.g., 150-1000$\mu$m) metal interlayers of joining ceramics, composites and other materials that are not easily welded or brazed using conventional processes. While such bonds can have high ultimate tensile strengths, it is shown that time-dependent failure of these bonds can occur at stresses (externally applied or residual) less than 20 percent of this value. These experiments also show that plastic deformation of the base metal accelerates rupture. Time-dependent failure appears to be caused by ductile rupture in the interlayer due to: (1) time-dependent creep of the interlayer if the base metal deforms only elastically or (2) time-dependent creep of the base metal (which induces time-dependent plasticity in the interlayer) if the base metal deforms plastically. In both cases, small ($\approx 10^{-3}$) plastic strains cause dislocation activity which leads to the nucleation of cavities that coalesce and cause failure.

The objective of this study was to help verify these theories using finite-element analysis. The results of these calculations are shown to be consistent with the delayed mechanical failure theory. For silver-interlayer bonds between elastic base metals, the dependence of the time-to-rupture on the calculated von Mises effective stress correlates well with the stress dependence for creep of pure silver. For bonds between plastic base metals, creep of the base metal is shown to induce time-dependent plasticity in the interlayer. Finally, calculations of the change in interlayer stress state with changes in the interlayer thickness and position correlate well with both the delayed failure theory and experiment.

Keywords: Metals, Welds, Fatigue

398. Constitutive and Failure Behavior of Metals at High Rates of Tensile Strain

FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. H. Gourdin, (415) 422-8093/FTS 532-8093

The results of electromagnetically launched expanding-ring experiments and conventional compression tests with oxygen free electronic (OFE) copper of grain size 10 to 200 $\mu$m are reported and analyzed in terms of the mechanical threshold stress (MTS) model. The activation energy for slip and the strain rate pre-exponential have been taken from the literature, both other model parameters are derived from the present data. We find that the hardening, $d\sigma/d\epsilon$, varies significantly with the strain rate, but is independent of the grain size. This implies that the grain size dependence, which is well described by a Hall-Petch relationship, much be assigned to the "structure" independent, or "athermal," component of the flow stress. The parameters associated with "recovery" are critical to the description of the high-temperature high-strain-rate ring data, and we find slightly different values than those in the literature. Overall the model provides an excellent description of the material behavior over a wide range of grain size, strain rate and temperature. In particular, it successfully reproduces the subtle interplay between temperature and strain rate that occurs during ring expansion. However, model calculations indicate that the plastic instability strain increases with increasing grain size, whereas observations of expanding rings show that the total elongation at failure increases with decreasing grain size. To resolve this apparent contradiction, we suggest that necks may grow more slowly in fine grained material.

Keywords: Metals, Expanding Rings, Constitutive Properties, Failure, High Strain-Rate

399. <u>Theoretical and Experimental Studies of Solid Combustion Reactions</u> <u>FY 1990</u>
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: J. B. Holt, (415) 422-8003/FTS 532-8003

Synchrotron radiation was used to study the formation of ceramic compounds by combustion synthesis. This process allowed characterization of the complex process that occurs as the combustion front proceeds at an extremely rapid rate. The results identified phase changes and chemical reactions not previously known.

Keywords: Combustion, Synchrotron Radiation

400. <u>Fracture Behavior of Refractory Metals and Alloys in Liquid Actinides</u>
<u>FY 1990</u>
$175,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: J. S. Huang, (415) 422-5645/FTS 532-5645

The effects of contact by liquid uranium (at 1200°C) on the tensile behavior of refractory metals dn alloys (such as Ta, W, Nb, V, Ta-W, and Nb-Ta) have been studied. The results showed that Ta, W, and Ta-W binary alloys are readily embrittled by liquid U, while Nb and V are not. For the Nb-Ta binary alloys, the embrittlement occurred in alloys which have more than 70 wt.% Ta. Metallographic and fracture surface examination indicated that the embrittlement in Ta, W, and Ta-W binary alloys is caused by localized grain boundary wetting of liquid U. It was found that the grain boundary wetting in these metal and alloys also occurred under stress-free conditions. The tendency for grain boundary wetting was also compared to calculated grain boundary energy and solid-liquid interfacial energy. It was found that the wetting was consistent with the energetic calculations, except for Nb and V for which the disagreement can be attributed to the large mutual solubilities between the solid and liquid elements.

To evaluate the possibility of embrittlement in Ta and W being caused by the classical LME mechanisms (i.e., adsorption of liquid atoms on solid causes reduction of interatomic bonding strength and subsequent brittle fracture), single crystals of W and Ta with orientation were tensile-tested in contact with liquid U. Only shallow penetration by liquid U was observed along dislocation slip planes. The specimens failed in a ductile manner, with no significant reduction of total elongation similar to the tests in vacuum. It can be concluded that a simple contact of liquid U is not sufficient to cause embrittlement of group VB and BTV metals and alloys.

Keywords: Deformation, Fracture, Actinide

401. Oxidation and Liquid Metal Resistant Coatings

FY 1990
$70,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: O. H. Krikorian, (415) 423-4655/FTS 543-4655

We have studied aluminide and silicide coatings for oxidation protection of Nb and Ta in fire environments, and oxysulfide coatings as protective coatings on V and Nb to provide for containment of molten U and Pu. The aluminides and silicides were applied by a slurry fusion process, while the oxysulfides were applied by evaporative deposition. Aluminide ($NbAl_3$) coatings on Nb are the best developed of these coatings and show good protection up to 1200°C. We have made a number of unique innovations in the coating process to enhance the coating performance as compared with ordinary intermetallic or ceramic coatings. For example, these coatings will self-heal and continue to provide good oxidation resistance even after microcracks are produced in the coatings by bending. The silicide coatings ($NbSi_2$ and $TaSi_2$) function well at temperatures of 1300-1800°C, but tend to fracture and fail in the 100-1300°C region. We have explored techniques whereby a low-melting low-viscosity oxide forms *in situ* and fills these fractures and provides oxidation protection in this 1001300°C regime without sacrificing coating performance at the higher temperatures. The oxysulfides (e.g., $Y_2O_2S$ and $Ce_2O_2S$) are advantageous as coating materials for containment of molten U because they are not wet by molten U up to ~1700°C and also show very little solubility or chemical interaction with molten U. This is the highest known temperature for which a material remains non-wetting toward molten U. Oxysulfide coatings have been successfully tested for containment of molten U up to 1400°C. Coatings tested with molten Pu have been limited to a temperature of only 100°C, but have shown similar behavior to U.

Keywords: Oxidation, Corrosion, Actinides

402. Development of Ultrafine Microstructures Through Rapid Solidification Rate Processing

FY 1990
$90,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: J. W. Elmer, (415) 423-4655/FTS 543-4655

Rapid solidification has resulted in the formation of a dispersion of ultrafine particles in dilute hyper-eutectic alloy systems. One system of interest is Al-Be, where Be particles form in an Al matrix at moderate-to-high solidification rates. These particles have a random crystallographic orientation and a unique modulated appearance, forming in "waves" parallel to the advancing solidification front. This microstructural pattern indicates that the Be particles periodically nucleate and grow from the liquid phase during non-steady-state solidification conditions. In Al 5 at.% Be, these particles form at solidification velocities on the order of 0.1 m/s and faster, and are on the order of 5 nm in diameter.

A rapid-solidification model has been developed to describe the formation of these particles. This model solves coupled differential equations to give the temperature, velocity, liquid composition, and the velocity-dependent partition coefficient of the rapidly-moving solid-phase front as a function of the transient solidification time. These parameters are then used to calculate the propensity for homogeneous nucleation of Be particles from the liquid ahead of the interface.

Keywords: Rapid Solidification

403. Failure Characterization of Composite Materials

FY 1990
$330,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: Scott Groves, (415) 422-1331/FTS 532-1331

We have characterized the three-dimensional performance of continuous fiber composite materials. This project has included data on three-dimensional failure and elastic properties as well as the dynamic strength behavior of these materials. Our accomplishments include the development of a unique multiaxial testing system for composite tubes, high strain rate testing fixtures, and enhancements to a drop tower for instrumented impact testing. We have also developed a three-dimensional orthtropic finite element code that will permit detailed ply-by-ply stress analysis.

Keywords: Composite Materials, Fibers, Failure Testing

404. Modeling Superplastic Materials

FY 1990
$260,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: Donald Lesuer, (415) 422-9633/FTS 532-9633

This project is developing a model that accounts for structural changes during superplastic flow and their subsequent influence on stress-strain behavior and deformation localization. We have studied the kinetics of strain-enhanced grain growth and cavitation and have assessed the ability of two rate dependent constitutive laws to predict the stress-strain behavior when the kinetics of microstructural evolution are included. The ability of instability criteria to predict strain localization during superplastic deformation has been assessed.

Keywords: Superplastic Flow, Deformation Modeling

405. Creep Model for Fiber Reinforced Epoxy-Resin Composites

FY 1990
$58,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: William W. Feng, (415) 422-8701/FTS 532-8701

A mathematical model of creep in a fiber reinforced epoxy-resin laminated composite has been developed. This model is based on composite micromechanics theory and uniaxial ply test data. A time-temperature correspondence principal has been used to evaluate the creep compliance for the epoxy resin. The predictions of the model will be compared against experimental test data on composite laminates. We plan to add this model to the NIKE3D structural program.

Keywords: Composite Materials, Creep Modeling

406. Superplastic Flow of Ceramics and Intermetallics

FY 1990
$125,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: E. N. C. Dalder, (415) 422-7270/FTS 532-7270

We are studying the superplastic behavior of $Si_3N_4$ and alloyed $Ti_3Al$ as functions of testing variables (strain rate and temperature) and starting microstructure. As part of this project we have developed an experimental apparatus capable of studying the mechanical response of ceramics to 200°C. We will be evaluating mechanisms that control superplastic flow in $Si_3N_4$ and alloyed $Ti_3Al$.

Keywords: Superplastic Flow, Ceramics

407. <u>Structural Joints for Composite Materials</u> FY 1990
$69,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: Frank Magness, (415) 423-1324/FTS 533-1324

This project is developing an accessible source of relevant information on composite joining combined with an empirically calibrated analytical capability which can be used for the specific design requirements of Laboratory programs. We have upgraded our current data base on composite joints including a baseline of practical experience in testing and evaluation of composite joints. We have also studied the correlation of empirical data and the results of finite element calculations.

Keywords: Composite Materials, Joining

408. <u>Interfaces, Adhesion, and Bonding</u> FY 1990
$380,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: Wayne E. King, (415) 423-6547

The influence of interfaces on materials properties is controlled by mechanisms that are operative over the range of length scales from atomic to macroscopic dimensions. Detailed determination of the operative mechanisms requires theory validated by comparable experiments. Theoretically, we have developed a unique capability for calculation of the electronic structure at interfaces, where symmetry is reduced compared with the bulk. Specifically, the method, called the real-space multiple-scattering theory (RSMST) can treat interfaces and include the effect of atomic relaxation at the interface. Currently, it is not possible to predict atomic relaxations using the RSMST (because of the large computational resources that would be required) so we have coupled this method with the semi-empirical embedded atom method (EAM) which uses modified two-body potentials with molecular dynamics, molecular statics, or Monte Carlo techniques to determine atomic rearrangements. These methods are at present limited to metallic systems; however, the extension of one or both methods to metal/ceramic interfaces appears to be possible.

Our experimental effort will produce results that are directly comparable with theoretical calculations. Consequently, our initial investigations will treat planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations relative to the perfect crystal. In order to span the entire range of length scales described above, macroscopic bicrystals a few millimeters thick, with interfacial areas on the order of a square centimeter will be required. In order to obtain such bicrystals, we plan to employ the diffusion bonding approach demonstrated at the Max-Planck-Institut, Institut für Werkstoffwissenschaft, Stuttgart, Germany (MPI). Initially, bicrystals are being obtained through a collaboration with MPI. An ultra-high-vacuum diffusion bonding machine will be developed in parallel with the proposed research project (in collaboration with Sandia National Laboratories-Livermore) for installation at LLNL.

Keywords: Interfaces, Bonding, Electronic Structure

Device or Component Fabrication, Behavior or Testing

409. IC Protective Coatings FY 1990
$720,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: M. Riley, (415) 422-2499/FTS 532-2499

We are developing coatings which are designed to protect the memory of ICs against intrusion and their architecture against reverse engineering. These materials must be capable of preventing easy access. We have fielded the first two generations of these materials. Current development efforts are devoted to the third and fourth generation coatings.

Keywords: IC Protection, Protective Coatings

410. Characterization of Solid-State Microstructures in High Explosives by Synchrotron X-ray Tomography FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. C. Tao, (415) 423-0499/FTS 543-0499

After demonstrating the feasibility of using 3D Microtomography to study pore distributions in materials with similar X-ray absorption coefficients as high explosives (HE), we have successfully applied the non-invasive techniques to characterize the detailed microstructures in HMX single crystals and a composite formulation consisting of fuel (RDX, NG/TA), oxidizer ($NaNO_3$), and metallic additives (aluminum). Due to cancellation of two dedicated runs at the Stanford Synchrotron Research Lab, we have performed the experiments using a conventional X-ray source coupled with the analytical software and data acquisition hardware developed for 3D Microtomography. Although the exposure time is lengthened and the spatial resolution is decreased slightly, we were able to resolve the topographical features of the HMX single crystal, the tomographical structure at a depth equal to 25 percent of the crystal thickness, and identify the aluminum and pore distribution in the composite mixture. The inability to probe the bulk of the HMX crystal for microstructural defects is due to beam hardening and penumbral blurring, both inherent technical inefficiency in a conventional X-ray source. With an intense source of monochromatic and tunable X-ray beam, such as that from a Synchrotron facility, we will be able to image the bulk crystal. The composite formulation examined supposedly was non-porous with the 5 $\mu$m aluminum dispersed evenly throughout the matrix. From our results, we found that the aluminum was not dispersed below a 50 $\mu$m scale, and the composition has approximately 5 percent porosity. This provided insights into the degree of mixing and wetting between components in the composite formulation as related to the formulation methodology. To further test our experimental capability, we designed a phantom matrix using the X-ray absorption coefficients for HMX,. with a complex integration of defect structures (pores, aluminum, orthorgonal microcracks, density gradients), and subjected this phantom for 3D Tomography analysis. Using a well characterized Synchrotron beam profile and the radiometric deconvolution techniques of our analytical software, we were able to reproduce the image of the phantom with minimal loss in structural resolution. This again demonstrates the capability of 3D Microtomography for examining defect microstructures in high explosives. These results were presented at the 9th Detonation Symposium at Portland, Oregon. The next phase of the research involves studying the correlation between microstructural defects and initiation sensitivity. Two experimental methods will be employed in this phase of the study: microphotography and infrared emission mapping. Coupled with both streak and frame cameras, ultrafast microphotography allows us to examine a single crystal under shock loading with a spatial and temporal resolution of 1 micron and 1 nsec, respectively. Measuring the infrared emission vs. time yields information on the mechanism of Hot-Spot formation and dissipation.

Keywords: Synchrotron, X-ray, High Explosive, Single Crystal, Initiation Sensitivity, Defect Microstructure, Non-Destructive Characterization

411. <u>Optical Diagnostics of High Explosives Reaction Chemistry</u> <u>FY 1990</u>
$175,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: R. L. Simpson, (415) 423-0379/FTS 543-0379

This research effort falls into two general technical areas: (1) high pressure deflagration of high explosives within a diamond anvil cell coupled with single shot coherent anti-Stokes Raman spectroscopy (CARS) designed to measure the pressure dependence of rapid decomposition and product formation and (2) using the spectral properties of Mie scattering to study time dependence and shock intensity sensitivity of the generation of sub-micron carbon particles in reacting high explosives and other energetic materials. Progress has continued in both areas from FY 1988. We have extended the burn rate curve of nitromethane to 40 GPa and have observed an interesting deuterium isotope effect on these rates in $CD_3NO_2$. Preliminary work has begun to extend this technique to HMX, RDX, and TATB. Seven shots were conducted on the scattering properties of shocked benzene. The timescales of the production of carbon particles as well as light absorbing molecular transients has been identified.

Keywords: Reaction Zone Chemistry, High Explosive Carbon Particle Formation, Time Resolved Diagnostics

## Instrumentation and Facilities

412. Scanning Tunneling Microscopy FY 1990
$320,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. Siekhaus, (415) 422-6884/FTS 532-6884

Scanning tunneling microscopy techniques in air were used to (1) deposit (by voltage pulse deposition) and to study the morphology of multimers (50-200 bases) of doublestranded DNA adsorbed on the basal plane of graphite, (2) to image with atomic resolution individual bases of DNA (Adenine, Thymine) adsorbed on graphite. The objective is to use scanning tunneling microscopy techniques to sequence DNA. Scanning tunneling microscopy in UHV was perfected, and used to study the morphology of metal clusters laser-deposited onto the surface of graphite and silicon.

Keywords: Instrumentation and Technique Development, Surface Structure, DNA Sequencing, Cluster, Laser Deposition

413. Scanning Tunneling Microscopy (STM) and Atomic Force Microscope (AFM) as a Detector FY 1990
$320,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: W. Siekhaus, (415) 422-6884/FTS 532-6884

One vibrating needle AFM, built in conjunction with LBL, capable of operating both as STM and AFM has been used to study the forces applied when scanning tunneling microscopy is being performed on biological molecules in air. A commercial AFM has been used to (1) study the structure of mouse, bull, and human sperm-heads, determining the packing density and packing morphology of DNA in sperm-heads, (2) to study the relationship between surface morphology and laser damage threshold of sapphire surfaces and of anti-reflection and high-reflection optical coatings.

Keywords: Instrumentation and Technique Development, Defects, NDE, Sperm, DNA, Laser Damage Threshold

414. Tritium Facility Upgrade

FY 1990
($7,800,000)*

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: J. H. Richardson, (415) 423-5187/FTS 543-5187

The Tritium Facility Upgrade (TFU) consists of three line items: (1) a new 5,700 square foot office addition along with modification of 2,000 square feet of the existing facility, (2) a Vacuum Effluent and Recovery System (VERS) designed to recover over 90 percent of the existing routine stack emissions, (3) a Secondarily Contained Tritium System (SCOTS) which replaces the existing low and high pressure systems with a modern totally secondarily contained system. This is designed to capture and then recover via VERS any accidental spill when handling large quantities of tritium.

Presently, the office addition is complete and has received final DOE acceptance. VERS design and construction is complete and is presently in the final acceptance testing phase. SCOTS is in final design stage with construction approximately 80 percent complete. Scheduled project completion is in February 1990.

Keywords: Facilities, Tritium

415. Decontamination and Waste Treatment Facility (DWTF)

FY 1990
($7,700,000)**

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LLNL Contact: R. Quong, (415) 422-7093/FTS 532-7093

Construction of the DWTF is scheduled to be completed by year-end 1992. The project started in FY86; through FY89, 19 percent of the $41.3 million authorized funds has been expended. Title 2 final design is complete. A draft environmental impact statement (DEIS) has been prepared and issued for public comment. Applicable permits (RCRA and Air Quality) have been submitted and have undergone initial review by the regulatory agencies. The progress of the environmental documentation and permits has been slowed by an ongoing internal review of the DWTF by the Laboratory. Some changes in the facility design is anticipated. The DWTF is a line-item construction project comprising seven new buildings

*Line-Item Construction Project: not included in subtotal or total.

**Line-Item Construction Project: not included in subtotal or total.

(88,000 square feet of new building space) plus a full complement of treatment equipment including a rotary kiln incinerator system. The facility will occupy a 6-acre site within the laboratory, replace existing outmoded facilities, and will greatly diminish the need for off-site treatment and disposal of waste generated by the laboratory.

Keywords: Facilities, Waste Treatment

Los Alamos National Laboratory

Materials Preparation, Synthesis, Deposition, Growth or Forming

416. Actinide Processing Development

FY 1990
$1,350,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: M. F. Stevens, (505) 667-4414/FTS 843-4414

The aim of this project is the development and characterization of fabrication processes and the study of new processing technologies for plutonium. Research involves casting, thermomechanical working, and stability studies. Measurements of resistivity, thermal expansion, magnetic susceptibility, and formability are made to evaluate fabrication processes and alloy stability.

Keywords: Radioactive Materials, Plutonium Alloys, Ductility, Thermal Expansion, Electrical Resistivity, Stability

417. Plutonium Oxide Reduction

FY 1990
$150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: K. Axler, (505) 667-4045/FTS 843-4045

The thermodynamics of interactions among the components used in the pyrochemical processing of plutonium are determined along with the relevant phase relations.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams, Direct Oxide Reduction, Electrorefining, Molten Salt Extraction

418. Ion-Beam Implantation FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

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

419. Electroplating Low Atomic Number Materials FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: T. Mayer, (505) 667-1146/FTS 843-1146

Aqueous solutions presently limit the metals that can be electroplated. This project is looking at electroplating low-atomic-number metals (aluminum and beryllium) by using non-aqueous plating baths. These new baths include solvents and fused salts. Applications include weapons components and inertial confinement fusion (ICF) target fabrication.

Keywords: Electroplating, Aluminum, Beryllium, Coatings, Metals

420. Liquid Crystal Polymer Development FY 1990
$300,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: R. Liepins, (505) 667-2656/FTS 843-2656

Conventional liquid crystal polymers possess high strength in only one direction. Working with theoretical physicists, an attempt are being made to synthesize a liquid crystal polymer with strength in three dimensions. This will be a unique polymer with a number of possible applications. Low to medium molecular weight polymers have been synthesized.

Keywords: Liquid Crystal Polymers

421. Low-Density, Microcellular Plastic Foams FY 1990
$250,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: J. Williams, (505) 667-7887/FTS 843-7887

Microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc are manufactured by a nonconventional foaming process. Foams are open-celled and have large surface areas. This process is being expanded to other polymeric materials for a wide variety of applications. Foams have cell sizes from 25um down to the 1um range depending on the process. Composite foams are being produced with submicron cell sizes while maintaining structural properties.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

422. Target Coatings FY 1990
$400,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: J. R. Laia, (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, Chemical Vapor Deposition

423. Physical Vapor Deposition and Surface Analysis FY 1990
$700,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: M. Scott, (505) 667-7557/FTS 843-7557

Physical vapor deposition and sputtering are employed to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers. Materials being developed include doped, *in situ* laminates of aluminum and $Al_xO_y$ having high strength and smooth surface finish. Also included are ion plating of aluminum and rare earth oxides onto various substrates for corrosion resistance to gases and liquid plutonium, deposition of oriented AlN onto various substrates is accomplished to enable nondestructive evaluation of materials, reflective and anti-reflective coatings for infrared, visible, ultraviolet and X-ray wavelengths. Novel photocathodes are being made and evaluated by these processes.

Keywords: Coatings and Films, Physical Vapor Deposition, Sputtering, Ion Plating, Corrosion, Nondestructive Evaluation

424. Chemical Vapor Deposition (CVD) Coatings — FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contacts: J. R. Laia and M. T. R. Kula, (505) 667-3239/FTS 843-3239

Chemical vapor deposition (CVD) techniques are used to deposit thin-film and bulk coatings of a wide variety of elements and compounds. Coatings are deposited by the following techniques: conventional flow-by, fluidized-bed, plasma-assisted, and chemical vapor infiltration. To support and enhance our basic CVD program, efforts are underway to study the fundamental nature of the CVD process, including *in-situ* diagnostics in the gas phase just above the substrate and modeling efforts to predict gas flows, reactor design, and chemical behavior within the CVD systems. Another collaborative effort at Los Alamos is attempting to synthesize organometallic precursors to deposit coatings at temperatures <300 °C. Substrates coated by the CVD technique range from particles 2.0 μm diameter to infiltrations of fabrics a square meter in area.

Applications include nuclear and conventional weapons, space nuclear reactor systems (fuels and structural components), inertial confinement fusion program, high temperature engine and structural components for advanced high-performance aircraft, hard/wear resistant coatings (tribological), corrosion resistant coatings, coatings of complex geometries, near-net-shape fabrication, heat-pipe structures, precision CVD of ultra-thin, freestanding shapes.

Keywords: Chemical Vapor Deposition, Coatings (metal and ceramic)

425. Polymers and Adhesives — FY 1990 $450,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: D. A. Hemphill, (505) 667-8335/FTS 843-8335

The objective of this project is to identify potential weapons engineering and physics applications for plastic and composite materials, select or develop appropriate materials, develop low cost fabrication techniques compatible with Integrated Contractor production capabilities, and to characterize promising materials on a timely basis to provide optimum material choices for new weapons designs. Material or process development projects include: highly filled polymers, composite structural and spring components, cushioning materials, and high-explosive compatible adhesives, potting materials, and castable loaded thermoplastics.

Keywords: Adhesives, Composites, Plastics, Polymers, Weapons Design, Weapons Engineering, Integrated Contractors

426. Tritiated Materials — FY 1990 $511,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
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 using laser-Raman techniques for *in situ* measurements or deuterium-tritium gas mixtures, and kinetic studies of hydrogen-metal interactions.

Keywords: Tritium, Metal Tritides, Li(D,T), Tritiated Materials, Radioactive Materials

427. Salt Fabrication — FY 1990 $379,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: D. H. W. Carstens, (505) 667-5849/ FTS 843-5849

Development and evaluation of new fabrication and containment processes for Li(D,T) (salt). Research topics include development of hot pressing, machining techniques for salt compacts, new containment methods, and studies of radiation induced growth and outgassing.

Keywords: Tritium, Hydrides, Machining, Radioactive Materials, Near-Net-Shape Processing

428. Slip Casting of Ceramics — FY 1990 $150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: G. F. Hurley, (505) 667-9498/FTS 843-9498

We are slip casting many ceramics including alumina, magnesia, and thoria. The technology uses colloidal chemistry and powder characterization theory along with materials engineering. Bodies so formed are used in many energy technologies including nuclear reactors. Development problems include processing of powder to yield satisfactory sintering and shrinkage. Success may lead to improved materials with superior strength. We are now investigating the use of this technology to form thermal-shock-resistant bodies from transformation-toughened ceramic alloys.

Keywords: Ceramics, Microstructure, Strength, Sintering Refractory Liners, Thoria, Transformation Toughened Ceramics, Thermal Shock

429. Glass and Ceramic Coatings

FY 1990
$40,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: R. E. Honnell, (505) 667-5432/FTS 843-5432

Components employing ceramic-metal seals, metallizing, and insulating coatings are fabricated for various groups associated with accelerator technology. Novel material applications are used to solve difficult electrical problems. Ceramic coated metals have been investigated for liquid metal containment.

Keywords: Enamels, Ceramic Coatings, Metals, Radiation Effects, Accelerator Technology

430. Cold Pressing, Cold Isostatic Pressing and Sintering

FY 1990
$10,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: G. F. Hurley, (505) 667-9498/FTS 843-9498

Cold pressing and cold isostatic pressing are used to consolidate ceramic and metal powders to support laboratory programs. Materials processed include $UO_2$, $ThO_2$, $Al_2O_3$, $Y_2O_3$, and MgO. End uses include plutonium processing hardware and fluxes, simulated fuel pellets, high temperature resistant ceramics for nuclear reactors.

Keywords: Cold Pressing, Sintering, Ceramics

431. Plasma-Flame Spraying Technology

FY 1990
$185,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
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

432. Rapid Solidification Technology — FY 1990 $100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
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

433. Microwave Sintering/Processing — FY 1990 $120,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: J. D. Katz, (505) 667-1424/FTS 843-1424

In this program, techniques of bonding and sintering ceramics are being investigated. Materials under study include $Al_2O_3$, $B_4C$ and $TiB_2$ as well as ceramic composites such $Al_2O_3$-SiC platelets. The method involves the use of 2.45 GHz microwaves which couple directly to the area in which the heat is needed. It has potential technical advantages related to heat distribution effects and a cost advantage because only the part is heated. Problems to be investigated include the control of the heating and its effect on microstructure.

Keywords: Ceramics, Sintering, Microwave Sintering, RF Heating

434. Predictions of Super Strong Polymers — FY 1990 $565,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: Flonnie Dowell, (505) 667-8765/ FTS 843-8765

Advanced, first-principles, microscopic, molecular statistical-physics theories have been originated and developed into mathematical models that have been used to predict (with the aid of computer-based modeling) new molecular structures most likely to form super strong polymers. These candidate molecules are being chemically synthesized and will be experimentally characterized. The theoretical work is continuing with emphasis on the prediction of other mechanical and dynamic properties, solvent effects, and processing conditions.

Keywords: Super Strong Polymers, Modeling

435. Synthesis of Ceramic Coatings

FY 1990
$30,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: C. P. Scherer, (505) 665-3202/FTS 855-3202

The objective of this effort is to synthesize Ceramic Films for liquid metal containment. Organic and aqueous solvents are of interest, but initial efforts have focused on nonaqueous. Film materials of interest include erbia, yttria, and magnesia.

Keywords: Ceramic Coatings, Sol Gel

436. Laser Surface Treatment of Materials

FY 1990
$250,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: D. V. Duchane, (505) 667-6887/ FTS 843-6887

Laser surface treatment of metals such as stainless steel and titanium coated stainless steel is being investigated. An excimer laser is used to briefly melt the top micron layer of the material. During this time diffusion and/or ion mixing takes place resulting in a change in surface properties without a deterioration of bulk properties.

Keywords: Laser Surface Treatment, Stainless Steel, Titanium Diffusion

Materials Structure or Composition

437. Actinide Surface Properties

FY 1990
$700,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: D. C. Christensen, (505) 667-2556/ FTS 843-2556

Characterization of actinide metal, alloy and compound surfaces using the techniques of X-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy. Surface reactions, chemisorption, attack by hydrogen, and the nature of associated catalytic processes are being studied.

Keywords: Actinides, Hydrides, Surface Characterization and Treatment, Hydrogen Effects, Radioactive Materials

438. Neutron Diffraction of Pu and Pu Alloys and Other Actinides — FY 1990 $237,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: A. C. Lawson, (505) 667-8844/FTS 843-8844

Physical structure and properties of plutonium are being studied by pulsed neutron diffraction at the Manuel Lujan, Jr., Neutron Scattering Center (Los Alamos) and the Intense Pulsed Neutron Source (Argonne). A time-of-flight technique is used to measure diffraction at cryogenic and elevated temperatures.

Keywords: Alloys, Radioactive Materials, Transformation, Microstructure

439. Surface, Material and Analytical Studies — FY 1990 $250,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: W. C. Danen, (505) 667-4686/FTS 843-4686

Studies are underway in four key areas: surface and interfacial structures and properties, explosives dynamics, laser-based isotopic analysis, and metastable energetic materials. Current investigations in surface and interfacial studies include: surface modification, HTSC composition and structure, and the use of MeV ion beams. In explosives chemistry, we are using real-time optical- and mass-spectral methods to probe the early-time dynamics of detonation. Analytical studies have centered on the use of resonance ionization mass spectrometry to eliminate isobaric interferences in the measurement of high-dynamic range isotope ratio measurements. During FY90 we initiated a study involving the synthesis and characterization of a new class of high energy density materials consisting of atomically-thin multilayerd composite materials.

Keywords: Surface, Explosives, Interfaces, Composite Materials

Materials Properties, Behavior, Characterization or Testing

440. Mechanical Properties of Plutonium and Its Alloys

FY 1990
$450,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: M. Stevens, (505) 667-4414/FTS 843-4414

The mechanical properties of plutonium and its alloys are related to the pre-test and post-test microstructures of the materials using optical and electron microscopy and X-ray, electron and neutron diffraction.

Keywords: Alloys, Radioactive Materials, Microstructures, Strength, Transformation

441. Phase Transformations in Pu and Pu Alloys

FY 1990
$450,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: M. Stevens, (505) 667-4414/FTS 843-4414

Mechanisms and crystallography of thermally and mechanically induced allotropic transformations are studied with differential scanning calorimetry, optical and electron microscopy and electron and X-ray diffraction.

Keywords: Alloys, Radioactive Materials, Microstructure, Transformations

442. Plutonium Shock Deformation

FY 1990
$350,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 3687
LANL (Contract No. W-7405-ENG-36) Contact: M. J. Reisfeld, (505) 667-1375/FTS 843-1375

Plutonium and actinide alloys are subjected to shock deformation, recovered without further damage and examined to determine how the shock affected their microstructures and mechanical properties.

Keywords: Radioactive Materials, Plutonium Alloys, Microstructure, Strength

443. Non-Destructive Evaluation FY 1990
$500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: M. Mathieson, (505) 667-6404/FTS 843-6404

Development of Nondestructive Evaluation Technology that produces quantitative estimates of material properties. Use of tomographic techniques to enhance radiographic inspection. In-process ultrasonic probing of plutonium bonding methods. Flash, cine radiography, high speed video recorded optical and X-ray diagnostics of dynamic and ultra-fast events. Real-time radiography. Image enhancement of output results from all techniques.

Keywords: Nondestructive Evaluation, Radiography, Ultrasonic Microscopy, Tomography, Cine Radiography, Bonding Processes, Real-Time Radiography, Image Enhancement

444. Powder Characterization FY 1990
$50,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: G. J. Vogt, (505) 667-5813/FTS 843-5813

Synthesis and processing of ceramic or metal powders critically depends on the physical characterization of the starting powders being used. Typical starting powders include commercial powders of thoria, silicon nitride, magnesia, alumina, tungsten, copper, and tungsten carbide. In the past year, considerable effort has been given to characterizing commercially prepared high-$T_c$ precursor powders and superconducting powders. Physical properties of interest include particle size and distribution, surface area, bulk and packed densities, morphology, pore size and distribution, and zeta potential. The crystalline-phase composition of the starting powders and processed powders can be determined by X-ray diffraction.

Keywords: Metal Powder, Ceramic Powder, Particle Size, Superconducting Powder, X-ray Diffraction, Surface Area

445. Shock Deformation in Actinide Materials FY 1990
$200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: M. Stevens, (505) 667-4414/FTS 843-4414

Measurement of shock-wave profiles in uranium, plutonium, and plutonium alloys. Use of soft-shock recovery test to examine the microstructural changes occurring during shock deformation. Measurement of spall strength in actinide materials and examination of fracture surfaces.

Keywords: Actinides, Shock Deformation, Microstructure, Spall Strength

446. Dynamic Mechanical Properties of Weapons Materials FY 1990
$225,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: G. Gray, (505) 667-5452/FTS 843-5452

Measurements of dynamic stress-strain and fracture behavior of materials used for nuclear weapons. Development of plastic constitutive relations.

Keywords: Dynamic, Strength, Fracture, Microstructure

447. Dynamic Testing of Materials for Hyper-Velocity Projectiles FY 1990
$100,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: G. T. Gray, III, (505) 667-4665/FTS 843-4665

Spall testing of high density materials. Microstructural characterization and fractography on spall fracture surfaces. Dynamic and quasi-static compression tests.

Keywords: Shock Deformation, Spall Strength, Microstructure, Strength

448. Mechanical Properties FY 1990
$300,000

DOE Contact: R. J. Gottschall, (301) 353-3428/FTS 233-3428
LANL (Contract No. W-7405-ENG-36) Contact: M. G. Stout, (505) 667-6750/FTS 843-6750

Basic studies of mechanical properties of metals. Multi-axial testing on pure metals and alloys. Measurement and prediction of texture development and its effect on stress-strain behavior. Constitutive model development and implementation in large-scale computer calculations. Correlation with microstructural characterization.

Keywords: Mechanical Properties, Texture, Strength, Microstructure, Constitutive Modeling

Device or Component Fabrication, Behavior or Testing

449. Radiochemistry Detector Coatings — FY 1990 $200,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: G. Reeves, (505) 667-4290/FTS 843-4290

Physical vapor deposition of metallic and nonmetallic coatings is employed for preparation of radiochemical detectors.

Keywords: Coatings and Films, Physical Vapor Deposition, Radiochemical Detectors

450. Target Fabrication — FY 1990 $1,500,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contact No. W-7405-ENG-36) Contact: L. Foreman, (505) 667-1846/FTS 843-1846
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

451. Filament Winder — FY 1990 $80,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 3687
LANL (Contract No. W-7405-ENG-36) Contact: C. Sadler, (505) 667-5262/FTS 843-5262

The Entec filament winder in MST-7 Plastics is a 4-axis computer-programmed machine with a winding envelope extending up to 4 feet in diameter and 10 feet in length. It is being utilized to wind circumferential or helical cylinders, cones, spheres, and closed-end vessels from a variety of fibers including glass, kevlar, carbon, tungsten, and aluminum oxide. The applications cover a host of programs from within the Laboratory as well as from outside agencies.

Keywords: Filament Winding Composites

452. Polymeric Laser Rods FY 1990
$150,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 3687
LANL (Contract No. W-7405-ENG-36) Contact: R. Hermes, (505) 667-6862/FTS 843-6862

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

453. High Energy Density Welding in Hazardous Environments FY 1990
$350,000

DOE Contact: C. B. Hilland, (301) 353-3687/FTS 233-3687
LANL (Contract No. W-7405-ENG-36) Contact: R. Patterson, (505) 667-4365/FTS 843-4365

High powder Nd/YAG lasers combined with fiber optic beam delivery systems have been evaluated for welding applications in hazardous environments. Applications include the manufacture of nuclear weapons components and nuclear power reactor repair. High quality structural welds have been achieved without exposing the operators or the welding power supplies to the hazardous environment.

Keywords: Laser Welding, Fiber Optic Beam Delivery, Hazardous Environments, Nuclear Applications

## OFFICE OF FOSSIL ENERGY

The mission of the Fossil Energy Program is to develop technologies that will increase domestic production of oil and gas or that will permit the Nation to shift from oil or gas to more abundant coal. Specifically, the Fossil Energy role is to develop technologies to support the following objectives:

- Provide a capability to convert coal to liquid and gaseous fuels;
- Increase domestic production of coal, oil, and gas;
- Ensure that current and new facilities that burn coal can do so in an economically viable and environmentally acceptable manner; and
- Allow more efficient and more economically attractive utilization of fossil energy resources.

The Fossil Energy activity includes fourteen major programs, which are grouped under seven program offices. One of these seven is the Advanced Research and Technology Development Program of the Office of Technical Coordination, which is the central point of contact for inquiries from universities concerning the Fossil Energy program.

Project execution and technical monitoring are administered in five energy technology centers and selected national laboratories.

### Office of Technical Coordination

### Fossil Energy AR&TD Materials Program

The objectives of the Advanced Research and Technology Development program are to assess and identify long-range advanced research needs in coal processing, fossil fuels utilization and extraction, materials, components, and instrumentation; to provide oversight of ongoing advanced research in fossil energy so as to ensure balance and proper priorities; to initiate and fund projects involving new, exploratory concepts or goal-oriented basic research; to manage the Materials Research and University Coal Research programs; and to provide policies for, and overview of, Fossil Energy-supported university activities. The Advanced Research and Technology Development program also is designed to provide an effective communications channel between the Fossil Energy program and academic institutions; to encourage these institutions to become involved in programs related to the DOE Fossil Energy mission; and to manage programs concerned with providing an adequate technical base for development of commercial construction materials and instrumentation for Fossil Energy pilot plants and demonstration plants.

The program supports workshops to identify research needs in all fossil energy technologies and manages selected training programs for faculty and students at Energy Technology Centers. The acronym PF designates that the project was provided funds in prior years.

Materials Preparation, Synthesis, Deposition, Growth or Forming

454. Fundamental Study of Aluminizing and Chromizing Processes — FY 1990 $99,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735

Ohio State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No.19X-SB154C) Contact: R. A. Rapp, (614) 292-6178

The purpose of this work is to conduct a study of aluminizing and chromizing of iron-base alloys which will lead to a fundamental understanding of these processes. Halide-activated processes will be studied. The work will provide the ability to specify pack compositions and conditions that will assure the deposition of corrosion-resistant coatings. The work will also provide specifications such as coating thickness, diffusion zone thickness, and elemental concentrations for corrosion-resistant coatings.

Keywords: Alloys, Corrosion, Coatings

455. Procurement of Advanced Austenitic and Aluminide Alloys — FY 1990 $49,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-840R21400, Martin Marietta Energy Systems, Inc.) Contact: R. R. Judkins, (615) 574-4572/FTS 624-4572

This task provides funds for the procurement of alloys necessary for alloy development and evaluation activities on the Fossil Energy AR&TD Materials Program.

Keywords: Alloys, Aluminides, Austenitic

456. Iron Aluminide Processing FY 1990
$34,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-840R21400, Martin Marietta Energy Systems, Inc.) Contact: R. R. Judkins, (615) 574-4572/FTS 624-4572

This task provides funds for the procurement of major equipment items necessary for iron aluminide development activities on the Fossil Energy AR&TD Materials Program.

Keywords: Alloys, Aluminides

457. Development of Iron Aluminides FY 1990
$382,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-840R21400, Martin Marietta Energy Systems, Inc.) Contact: C. G. McKamey, (615) 574-6917/FTS 624-6917

The objective of this project is to develop low-cost and low-density intermetallic alloys based on $Fe_3Al$ with an optimum combination of strength, ductility, and corrosion resistance for use as components in advanced fossil energy conversion systems.

Keywords: Alloys, Aluminides

458. Welding Processing FY 1990
$34,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-840R21400, Martin Marietta Energy Systems, Inc.) Contact: R. R. Judkins, (615) 574-4572/FTS 624-4572

This task provides funds for the procurement of major equipment items necessary for welding activities associated with alloy development projects on the Fossil Energy AR&TD Materials Program.

Keywords: Alloys, Aluminides, Welding

459. Development and Evaluation of Advanced Austenitic Alloys FY 1990
$257,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. W. Swindeman, (615) 574-5108/FTS 624-5108

The purpose of this project is to evaluate austenitic alloys for improved performance in high-temperature components in advanced heat recovery and hot-gas cleanup systems. Detailed alloy performance criteria for advanced steam cycle alloys have been established. Factors considered included strength, ductility, corrosion resistance, high-temperature stability, and fabricability. The availability and performance of existing and emerging alloys were compared with the criteria and four alloy groupings were identified. The four groupings were (1) lean stainless steels containing <20 percent chromium, (2) iron-bearing alloys containing 20-30 percent chromium, (3) nickel-base alloys, and (4) aluminum/silicon-bearing alloys. The lean stainless steels were selected for further study, and industrial subcontractors supplied pilot heats of this alloy, a modification of type 316 stainless steel. Work to optimize the composition and heat treatment and studies of fabrication methods, joining methods, and surface treatments were undertaken. With the near completion of work on the lean stainless alloys, attention has turned to the 20-30% Cr alloys. Evaluation of the higher chromium alloys has been extended to temperatures of interest to PFBC hot-gas cleanup systems.

Keywords: Steam Cycle, Materials, Mechanical Properties, Austenitics, Hot-Gas

460. Evaluation of the Fabricability of Advanced Austenitic Alloys FY 1990
$26,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Babcock & Wilcox (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 72X-SB775C) Contact: M. J. Topolski, (216) 829-7301

The purpose of this work is to evaluate the fabricability, weldability, and surface treatments of advanced austenitic tubing for superheater applications. The problem of the fabrication of tubing from alloys containing controlled amounts of minor element additions and surface treatments of the tubing for optimum strength and corrosion resistance is examined in this activity.

Keywords: Austenitics, Alloys, Tubing

461. The Influence of Processing on Microstructure and Mechanical Properties of Aluminides | FY 1990 $173,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570) Contact: R. N. Wright, FTS 583-6127

The purpose of this project is to determine the influence of processing on the properties of alloys based on $Fe_3Al$. Thermomechanical processing is pursued to improve their room-temperature ductility. The response of the microstructure to annealing will be characterized in terms of the establishment of equilibrium phases and degree of long-range order. The mechanical properties are determined at room and elevated temperatures and related to the microstructure.

Keywords: Aluminides, Processing, Microstructure

462. Evaluation of the Fabricability of Iron Aluminides | FY 1990 $25,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
University of Pittsburgh (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Subcontract No. 19X-SF774V Contact: H. D. Brody, (412) 624-9724

The purpose of this project is to evaluate and improve the casting characteristics of iron aluminides. The following melting and casting characteristics will be evaluated: (1) the susceptibility of iron aluminide compositions to dissolution of hydrogen and oxygen during melting, pouring, and flowing through molds, (2) the influence of hydrogen and oxygen on microporosity and surface quality of iron aluminide compositions, (3) the melt fluidity and its dependence on composition, superheat, metal head, and mold material, (4) hot-tearing susceptibility and its dependence on composition and superheat, (5) the influence of composition and superheat on as-cast grain size, (6) the ability to feed solidification shrinkage through standard foundry technique, and (7) the influence of casting parameters on tensile properties.

Keywords: Aluminides, Fabricability, Casting

463. Investigation of Electrospark Deposited Coatings for Protection of Materials in Sulfidizing Atmospheres FY 1990 $106,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Westinghouse Hanford Company (FWP ERT0001) Contact: R. N. Johnson, (509) 376-3582

The purpose of this task is to examine the use of the electrospark deposition coating process for the application of corrosion-, erosion-, and wear-resistant coatings to candidate superheater alloys. Materials to be deposited may include MCrAl, MCrAlY, highly wear-resistant carbides, and other hardsurfacing materials.

Keywords: Coatings, Materials

464. Vapor-Liquid-Solid SiC Whisker Process Development FY 1990 $99,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Los Alamos National Laboratory (Contract No. W-7504-eng-36) Contact: J. D. Katz, (505) 665-1424/FTS 855-1424

The purpose of this project is to provide assistance in transferring the laboratory-scale Vapor-Liquid-Solid (VLS) SiC whisker growth process to an industrial organization for engineering-scale development.

Keywords: Ceramics, Whiskers, Composites

465. Ceramic Composite Processing FY 1990 $35,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-840R21400, Martin Marietta Energy Systems, Inc.) Contact: R. R. Judkins, (615) 574-4572/FTS 624-4572

This task provides funds for the procurement of major equipment items necessary for ceramic composite development and characterization activities on the Fossil Energy AR&TD Materials Program.

Keywords: Ceramics, Composites

466. Fabrication of Fiber-Reinforced Composites by Chemical Vapor Infiltration and Deposition (CVID) FY 1990 $188,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: D. P. Stinton, (615) 574-4556/FTS 624-4556

The purpose of this task is to develop a process for the fabrication of fiber-reinforced ceramic composites having high fracture toughness and high strength. This process utilizes a steep temperature gradient and a pressure gradient to infiltrate low-density fibrous structures with gases, which deposit as solid phases to form the matrix of the composite. Modifications to the process which are being explored include controlling the porosity and permeability of the fibrous preforms and variation of the deposition conditions. Alternate matrices, alternate fiber types, and pretreating or coating of fibers will be investigated to optimize the mechanical properties of the composites.

Keywords: Composites, Fiber-Reinforced, Ceramics

467. Characterization of Fiber-CVD Matrix Interfacial Bonds FY 1990 $138,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. A. Lowden, (615) 574-7714/FTS 624-7714

The purpose of this task is to optimize the strength and toughness of fiber-reinforced ceramic composites by tailoring the strength of the bonds between the fiber and the matrix. Methods must first be developed to characterize the fiber-matrix bond strengths in fiber-reinforced ceramic composite systems. Coating or pretreatment processes can then be utilized to tailor the fiber-matrix bonding within various composite systems and to optimize the strength and toughness of the composite.

Keywords: Composites, Ceramics, Fiber-Reinforced, Interfaces

468. Microwave Sintering of Ceramics FY 1990
$197,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: M. A. Janney and H. D. Kimrey, (615) 574-4281/FTS 624-4281

The purpose of this activity is to explore the feasibility of using microwave heating as a means of fabricating electrode, electrolyte, and interconnect materials having improved electrical properties for monolithic solid oxide fuel cell design being advanced by Argonne National Laboratory. The ultimate goal is to develop the technology (materials and process) for fabricating a complete monolithic fuel cell module in one operation.

Keywords: Ceramics, Microwave Sintering, Fuel Cells

469. Development of Advanced Fiber Reinforced Ceramics FY 1990
$148,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Georgia Institute of Technology, Georgia Tech Research Institute (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-43369C) Contact: T. L. Starr, (404) 894-3678

The purpose of this research effort is to conduct a theoretical and experimental program to identify new compositions and processing methods to improve the physical and mechanical properties of selected fiber-reinforced ceramics. The ceramic matrix material is amorphous fused silica or modified silica glass, and the focus is the development of fiber-reinforced silica. Parameters studied include: (1) differences in elastic modulus between matrix and fiber, (2) differences in thermal expansion, (3) nature of interfacial bond, (4) densification of matrix, (5) nature of fiber fracture/pull-out, (6) fiber diameter and fiber length-to-diameter ratio, (7) fiber loading, and (8) fiber dispersion and orientation. A model will be developed based on the information generated in the experimental phase of the program.

Keywords: Ceramics, Composites, Fiber-Reinforced

470. Modeling of Fibrous Preforms for CVD Infiltration FY 1990
$49,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Georgia Institute of Technology, Georgia Tech Research Institute (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-55901C) Contact: T. L. Starr, (404) 894-3678

The purpose of this project is to conduct a theoretical and experimental program to develop an analytical model for the fabrication and infiltration of fibrous preforms. Chemical vapor deposition (CVD) has demonstrated considerable promise as a technique for fabrication of fiber-reinforced ceramic composites. Unidirectional and cloth-reinforced composites of SiC fibers in a SiC matrix have shown good strength and exceptional strain tolerance. However, results have been inconsistent with the fabrication of randomly oriented short-fiber composites. A critical problem has been the inability to consistently fabricate fibrous preforms with both high fiber loading and a permeability suitable for infiltration. A better understanding of the fundamental parameters controlling preform fabrication and CVD infiltration of such preforms is needed to guide further development. The proposed analytical model will: (1) predict preform structure (density, porosity, fiber orientation, etc.) based on fabrication technique and fundamental fiber parameters (diameter, aspect ratio, etc.), and (2) predict permeation and heat conduction through the preform structure and, thus, predict the CVD infiltration performance. Initially, the model will be developed for preforms containing only one type of fiber, but extension to mixed fiber and fiber-particle blends is planned.

Keywords: Ceramics, Composites, Modeling

471. Electroslag Casting Technology Transfer FY 1990
$148,000

DOE Contacts: V. Kothari, FTS 923-4505 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: V. K. Sikka, (615) 574-5112/FTS 624-5112

The purpose of this project is to transfer the electroslag casting technology for iron aluminides to industry. The technology transfer will be carried out using the ductile, ordered iron aluminide alloys and will be limited to simple shapes such as rounds and slabs. The rounds and slabs will be tested in the as-cast and wrought conditions. Experience with simple shapes will be extendable to more complex shapes with changing section sizes.

Keywords: Casting, Electroslag

Materials Structure and Composition

472. Analytical Characterization of Coal Surfaces and Interfaces FY 1990
$279,000

DOE Contacts: J. D. Hickerson, FTS 723-5721 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, and Inc.) Contact: V. J. Tennery, (615) 574-5124/FTS 624-5124

The objective of this task is to provide analytical characterization of coal surfaces and interfaces between coal and various included minerals for the purpose of assisting the Pittsburgh Energy Technology Center in its research on coal characterization and cleaning. Particular emphasis is given to the chemical binding of the detrimental elements, including sulfur, nitrogen, mineral matter, etc. The distribution of these elements in various coals, and particularly the chemical and structural characterization of interfaces in coals are major tasks in the research.

Keywords: Coal, Surfaces, Interfaces

Materials Properties, Behavior, Characterization or Testing

473. Transfer Model Predicting Thermomechanical Behavior of Refractory Linings to Industry FY 1990
$82,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Tennessee Center for Research and Development (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 41X-SB628V)
Contact: A. H. von der Esch, (615) 675-9505

The purpose of this activity is to develop user-friendly and intelligent computer-based software for the prediction of thermomechanical behavior of refractory lining systems. The user-friendly software system is anticipated to enable users to have access to design guidelines and to develop preliminary refractory designs, to perform finite element analyses for final designs, and to facilitate the modification of existing or the addition of new capabilities through a modular program structure.

Keywords: Refractory Linings, Software, Stress Analysis

474. Mechanical Properties and Microstructural Stability of Advanced Austenitic Alloys

FY 1990
$138,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Cornell University, Materials Science and Engineering Department (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-27488C) Contact: Che-Yu Li, (607) 255-4349

The purpose of this project is to rank the strengths and metallurgical stabilities of advanced austenitic alloys at temperatures ranging from 650° to 760°C. Mechanical testing of the steels consists of relaxation experiments (24 h duration each) that cover stresses producing deformation rates from about $10^{-3}$ to $10^{-9}$/sec. The precipitate or dislocation microstructure of the steels in the grain boundary and matrix regions is being studied to determine the role of strain-time history on the stability of the microstructure. The relaxation data will be correlated with constant-load creep data provided by Oak Ridge National Laboratory and analyzed in terms of deformation mechanisms to determine relative contributions of grain boundary and matrix deformations. The most promising alloys from the screening test will be included in relaxation tests at 700°C to determine optimum heat treatments for strength and metallurgical stability.

Keywords: Steam Cycle, Microstructure, Mechanical Properties

475. Investigation of the Weldability of Iron Aluminides

FY 1990
$74,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Colorado School of Mines, Center for Welding Research (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-27421C) Contact: G. R. Edwards, (303) 273-3773

The purpose of this project is to study the weldability of 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.

Keywords: Joining, Welding

476. Aqueous Corrosion of Iron Aluminides FY 1990
$49,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Tennessee (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 41B-07685C) Contact: R. A. Buchanan, (615) 974-4858

The objective of this project is to investigate the aqueous corrosion of iron aluminides based on $Fe_3Al$. The effort will provide basic corrosion information over a wide range of pH values for each of several experimental iron aluminide compositions and will allow comparisons to be made among iron aluminide compositions, as well as with other corrosion-resistant materials of interest to fossil energy systems.

Keywords: Alloys, Aluminides, Corrosion

477. Fireside Corrosion Tests of Candidate Advanced Austenitic Alloys, Coatings, and Claddings FY 1990
$0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Foster Wheeler Development Corporation (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-SA187C) Contact: J. L. Blough, (201) 535-2355

The purpose of this project is to provide comprehensive corrosion data for selected advanced austenitic tube alloys in simulated coal ash environments. ORNL-modified alloys and standard comparison alloys will be examined. The variables affecting coal ash corrosion and the mechanisms governing oxide breakdown and corrosion penetration will be evaluated. Corrosion rates of the test alloys will be determined as functions of temperature, ash composition, gas composition, and time. The parameters influencing corrosion rates will be identified and correlated with past data for high temperature alloys.

Keywords: Austenitics, Alloys, Corrosion

478. Joining Techniques for Advanced Austenitic Alloys FY 1990
$148,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Tennessee (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 41B-07685C) Contact: C. D. Lundin, (615) 874-5310

Weldability is an important consideration in the selection of a suitable alloy for the fabrication of boiler components such as superheaters and reheaters. It is often a challenge to select joining materials and establish procedures that will allow advanced materials to function at their full potential. The purpose of this research is to examine important aspects of newly developed austenitic tubing alloys intended for service in the temperature range 550° to 700°C.

Keywords: Alloys, Austenitics, Joining, Welding

479. Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments FY 1990
$316,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Argonne National Laboratory (Contract No. W-31-109-eng-38) Contact: K. Natesan, (312) 972-5103/FTS 972-5103

The purposes of this task are to (1) evaluate the corrosion mechanisms for chromia- and alumina-forming alloys in mixed-gas environments, (2) develop an understanding of the role of several microalloy constituents in the oxidation/sulfidation process, (3) evaluate transport kinetics in oxide scales as functions of temperature and time, (4) characterize surface scales that are resistant to sulfidation attack, and (5) evaluate the role of deposits in corrosion processes.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

480. Environmental Effects on Iron Aluminides FY 1990
$192,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: J. H. DeVan, (615) 574-4451/FTS 624-4451

The purpose of this task is to develop protective oxide scales on $Al_20_3$-forming iron-based alloys in mixed oxidant environments. Important objectives include

(1) determination of the effects of sulfur on oxide microstructures, diffusion processes in the oxide, and nucleation and growth of sulfides, (2) examination of the effects of reactive elements on oxide properties in sulfur-containing environments, and (3) study of the mechanisms of both chemical and mechanical breakdown of oxide scales in mixed-gas atmospheres.

Keywords: Corrosion, Aluminides, Mixed-Gas, Scales

481. Secondary-Ion Mass Spectrometry Study of Scales on Iron Aluminides FY 1990
$15,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
AEA Industrial Technology, Harwell Laboratory (England)
(Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 90X-SF559V) Contact: Hugh Bishop

The purpose of this work is to analyze scales on iron aluminide alloys to determine the preferred diffusion paths of oxygen in these alloys.

Keywords: Scales, Aluminides

482. Investigation of Moisture-Induced Embrittlement of Iron Aluminides FY 1990
$59,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Rensselaer Polytechnic Institute (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-SF521C) Contact: N. S. Stoloff, (518) 276-3476

The purpose of this work is to study hydrogen embrittlement of iron aluminide alloys. Recently, it was demonstrated that the moisture in air can significantly reduce the room temperature tensile ductility of $Fe_3Al$-based alloys by apparently combining with the aluminum in the alloys and forming atomic hydrogen. This atomic hydrogen diffuses rapidly into the material causing embrittlement. It is very important to the development and future application of these alloys that the mechanism causing this embrittlement be understood. Experiments will be conducted on selected $Fe_3Al$ alloys that will lead to an understanding of the phenomenon. The work shall focus on effects of moisture on relevant mechanical properties such as fatigue and tensile strengths, and shall correlate important microstructural variables such as degree of order, grain size, phases present, etc., with the alloy's susceptibility to embrittlement. The hydrogen permeation through the alloy shall also be measured. Finally, the results of the experimental work shall be evaluated and summarized in a way that will attempt to define the mechanism of the embrittlement.

Keywords: Aluminides, Embrittlement, Moisture

483. The Effect of Alloying Constituents and Control of the Growth of Protective Oxide Scales — FY 1990 $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Battelle Columbus Laboratories (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-57444C) Contact: I. G. Wright, (614) 424-4377

The objectives of this program are: (1) to gain an improved understanding of the effects of alloying constituents present at low levels on the development and mode of breakdown of protective oxide scales in conditions representing those encountered in combustion and gasification processes, and (2) to achieve better control over the growth of scales which will contribute to improvements in long-term high-temperature corrosion resistance of heat exchanger and heat recovery materials.

Keywords: Corrosion, Oxides, Scales

484. Effect of Reactive Element Additions on the Protectiveness of Oxide Scales Formed in Sulfur-Containing Atmospheres — FY 1990 $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Case Western Reserve University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-95900C) Contact: K. M. Vedula, (216) 368-4211

The focus of the current program is to obtain a better understanding of material behavior in fossil energy environments. The particular emphasis is on the effects of reactive element additions on the protectiveness of oxide scales formed in sulfidizing/oxidizing atmospheres. Iron-based alloys, including Fe-25Cr and Fe-25Cr-20Ni which are $Cr_2O_3$ formers and Fe-25Cr-6Al which is an $Al_2O_3$ former, are the base alloys for this investigation. Conventional alloying as well as ion-implantation are the techniques for incorporating the reactive elements into the base alloys.

Keywords: Corrosion, Oxides, Scales

485. Effects of Several Variables on the Growth and Breakdown of Protective Alumina or Chromia Scales in Mixed-Gas Environments — FY 1990 $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Universal Energy Systems, Inc. (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 86X-95901C) Contact: V. Srinivasan, (513) 426-6900

The main objective of this program is to develop a comprehensive basic understanding of the effects of additions of microalloy constituents and the surface conditions on the nucleation, growth and breakdown of protective oxide scales in the mixed oxidant environments relevant to coal utilization and conversion technologies. The alloys of primary interest are ferritic and austenitic steels with adequate high temperature mechanical strength. Model alloy systems of such compositions that will develop protective chromia or alumina scales will be used. The scope of this program includes the study of the influence of the type and concentration of microalloying additions, the surface pretreatments, the method of incorporation of the microalloy constituents, the temperature and the partial pressures of oxygen and sulfur on the formation and degradation of scales. The temperature range of present interest is between 500° and 700°C. A variety of analytical tools will be used to characterize the scale and the substrate as a function of time of exposure to understand the distribution and chemical status of reactants in the pre- and post-exposed samples, so that degradation mechanism can be understood. Thermogravimetric and scales thickness measurements will be used to describe the kinetics under isothermal and cyclic conditions.

Keywords: Corrosion, Oxides, Scales

486. Molten Salt-Induced Corrosion of Iron Aluminides — FY 1990 $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
University of Cincinnati (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 19X-SD169V) Contact: R. Y. Lin, (513) 556-3116

The purpose of this project is to evaluate the molten salt-induced hot corrosion of nickel iron and iron aluminides. The use of nickel iron aluminides in fossil energy conversion and utilization systems requires resistance to mixed sulfidation/oxidation attack and severe corrosion in the presence of molten salts at elevated temperatures.

Keywords: Corrosion, Molten Salts, Aluminides

487. A Study of Erosive Particle Rebound Parameters FY 1990
$0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

University of Notre Dame (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc. Subcontract No. 19X-91236C) Contact: T. H. Kosel, (219) 239-5642

This research project is designed to provide a systematic investigation of the effects of materials properties and experimental variables on the rebound directions and velocities of erodent particles. The general approach is to develop computer models for the impact of spherical and angular particles, and to compare the predictions with experimental measurements of both single and multiple impact rebound parameters.

Keywords: Erosion, Wear, Particles

488. Studies of Materials Erosion in Coal Conversion and Utilization Systems FY 1990
$247,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Lawrence Berkeley Laboratory (Contract No. DE-AC03-76SF00098) Contact: A. V. Levy, (415) 486-5822/FTS 451-5822

The erosion of materials surfaces by small solid particles carried in gas and liquid streams is being investigated. The materials are tested over a range of conditions that simulate portions of the operating environments of containment surfaces in coal gasification, liquefaction, and fluidized-bed combustion processes. The effects of the materials properties, microstructures, and compositions on their erosion behavior are determined. The effects of elevated temperature corrosion in combination with the erosion are studied to determine the mechanisms and rates of the combined surface degradation modes.

Keywords: Corrosion, Erosion, Wear

489. Response of Metallic and Oxide Surfaces to Deformation FY 1990
$192,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: J. R. Keiser, (615) 574-4453/FTS 624-4453

This work consists of two subtasks related to the deformation response of metallic and oxidized surfaces. Subtask 1 is focused on the study of the erosion, corrosion, and erosion-corrosion of alloys to improve the understanding of the processes involved and the properties of materials that affect such behavior. The objective of Subtask 2 is to investigate the relationships between alloy composition and micromechanical properties of oxide scales to develop a methodology for designing improved (slow-growing, adherent, sound) scales on high-temperature alloys.

Keywords: Erosion, Wear, Corrosion, Metals, Alloys

490. Study of Particle Rebound Characteristics and Material Erosion at High Temperatures — FY 1990 $109,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
University of Cincinnati (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-89628C) Contact: W. Tabakoff, (513) 475-2849

The purpose of this effort is to investigate the erosion processes and fluid mechanics phenomena that occur in fluidized-bed combustors, coal-fired boilers, cyclones, pumps, turbines, valves, and other coal combustion systems. The overall objective is to develop a quantitative model that will facilitate the prediction of erosion in systems operating in particle-laden environments. This investigation will at first be limited to ductile target materials. The experimental study of the impact and rebound characteristics will be performed with selected solid particles, possibly $Al_2O_3$ and $SiO_2$. The target materials will be selected according to present and anticipated materials needs of coal combustion systems.

Keywords: Erosion and Wear, Corrosion, Metals, Alloys

491. Development of Nondestructive Evaluation Methods and Effects of Flaws on the Fracture Behavior of Structural Ceramics — FY 1990 $311,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Argonne National Laboratory (Contract No. W-31-109-eng-38) Contacts: W. A. Ellingson, (312) 972-5068/FTS 972-5068 and J. P. Singh, (312) 972-5132/FTS 972-5132

The purpose of this project is to study and develop acoustic and radiographic techniques and possible novel techniques such as nuclear magnetic resonance, to characterize structural ceramics with regard to presence of porosity, cracking, inclusions, amount of free silicon, and mechanical properties, and to establish the type and character of flaws that can be found by nondestructive evaluation (NDE) techniques. Both fired and unfired specimens will be studied, and correlations between NDE results and failure of specimens will be established.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

492. Joining of Silicon Carbide Reinforced Ceramics FY 1990
$173,000
DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570)
Contact: B. H. Rabin, FTS 583-0058

The purpose of this project is to explore and develop joining techniques for silicon carbide fiber-reinforced silicon carbide ceramics produced by chemical vapor infiltration and deposition (CVID). The research goals include identifying appropriate joining methods, establishing experimental procedures for fabricating joints, and characterizing the structure and properties of joined materials. An understanding of the factors that control joint performance will be obtained through studies of the relationships among processing variables, joint microstructures, and mechanical properties. The thermal and environmental stability of joints will be examined.

Keywords: Joining, Ceramics, Composites

493. Nondestructive Evaluation of Advanced Ceramic Composite Materials FY 1990
$172,000
DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Idaho National Engineering Laboratory (Contract No. DE-AC07-76ID01570)
Contact: L. A. Lott, FTS 583-6436

The purpose of this project is to develop an effective capability for nondestructive evaluation of ceramic fiber reinforced ceramic composites. The response of selected samples of sintered composite materials consisting of SiC fibers in SiC and $Si_3N_4$ matrices to both ultrasonic and radiographic techniques will be investigated. Experimental techniques and signal processing algorithms will be developed for: (1) characterizing acoustic properties and sample morphology, including fiber size and distribution and the degree of bonding of the fibers to the matrix, (2) detecting flaws including cracks, porosity, fiber clusters, and bonding anomalies, and (3) detecting flaws in joints. The NDE techniques developed in this project will result in more effective and extensive use of advanced ceramic composite materials in fossil energy applications.

Keywords: Ceramics, Composites, Nondestructive Evaluation

494. Structural Reliability and Damage Tolerance of Ceramic Composites FY 1990 $148,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

National Institute of Standards and Technology (Contract No. DE-A105-80OR20679) Contact: E. R. Fuller, (301) 975-5795

The objective of this study is to characterize the high temperature failure mechanisms and factors that influence their operation with an aim toward improving the properties of structural ceramics, especially silicon carbide and silicon nitride based materials, for use in coal conversion applications.

Keywords: Ceramics, Materials Characterization

495. Mechanical Properties of Ceramic Fiber-Ceramic Matrix Composites FY 1990 $91,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

North Carolina A&T State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-SC423C) Contact: J. Sankar, (919) 334-7620

The purpose of this project is to expand the mechanical properties data base for composites fabricated by forced chemical vapor infiltration (CVI). Composites are currently being fabricated with continuous SiC fiber reinforcement, SiC whisker reinforcement, SiC platelet reinforcement, and continuous aluminosilicate fiber reinforcement. The mechanical properties vary with the type of reinforcement and with the type of coating utilized to control the fiber/matrix interfacial bond. The effect of the reinforcement type and interfacial bond on the tensile strength, thermal shock resistance, oxidation resistance, and tensile strength during cyclic loading are investigated.

Keywords: Ceramics, Composites, Mechanical Properties

496. Ceramic Catalyst Materials: Hydrous Metal Oxide Ion Exchange Supports for Direct Coal Liquefaction FY 1990 $197,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Sandia National Laboratory (Contract No. DE-ACO4-76DP00789) Contact: D. H. Doughty, FTS 845-8105

This project involves investigation of the role of ceramic materials properties in the activity and selectivity of novel catalytic materials. The research focuses on the relationship between the catalytic activity and the composition, structure, and acid/base character of the ceramic support material.

Keywords: Ceramics, Catalysts

Device or Component Fabrication, Behavior or Testing

497. *Materials and Components in Fossil Energy Applications* (Newsletter) FY 1990 $114,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

Battelle-Columbus Laboratories (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 11X-78931C) Contacts: E. E. Hoffman (DOE/ORO), (615) 576-0735/FTS 626-0735 and I. G. Wright (BCL), (614) 424-4377

The purpose of this task is to publish a periodic (bimonthly) newsletter to address current developments in materials and components in fossil energy applications.

Keywords: Materials, Components

498. Mechanisms of Galling and Abrasive Wear FY 1990 $74,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735

National Institute of Standards and Technology (Contract No. DE-A105-83OR21322) Contact: L. K. Ives, (301) 975-6013

This project is directed to developing an understanding of the wear mechanisms of materials associated with valves in coal conversion systems. This work addresses the mechanical and chemical effects experienced in closure regions of valves in coal conversion systems. It includes theoretical considerations of chemical reactions and effects of the working media on valve closure materials. Measurements are being performed to determine the static and kinetic coefficients of friction of the various combinations of test materials.

Keywords: Erosion, Wear

499. Fabrication of Full-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition — FY 1990, $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
3M Company (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 93X-SB482C) Contact: T. Kafka, (612) 733-8065

The purpose of this project is to scale-up the chemical vapor infiltration and deposition (CVID) process developed at Oak Ridge National Laboratory for fabricating ceramic fiber-ceramic matrix composites. The goal is to use the scaled-up CVID process to produce composite filters that have the requisite strength and toughness, but which also have sufficient porosity to be permeable to gas streams and the appropriate size and distribution of porosity to be an effective filter. A practical process for fabricating porous ceramic fiber-ceramic matrix candle filters (full-size) with increased surface area will be developed.

Keywords: Ceramics, Composites, Filters

500. Development of Ceramic Membranes for Gas Separation — FY 1990, $327,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge Gaseous Diffusion Plant (Contract No. DE-AC05-84R21400, Martin Marietta Energy Systems, Inc.) Contact: D. E. Fain, (615) 574-9932/FTS 624-9932

The purpose of this activity is to fabricate inorganic membranes for the separation of gases at high temperatures and/or in hostile environments, typically encountered in fossil energy conversion processes such as coal gasification. This work is performed in conjunction with a separate research activity that is concerned with the development and testing of the ceramic membranes.

Keywords: Ceramics, Membranes, Filters, Separation

501. Investigation of the Mechanical Properties and Performance of Ceramic Composite Components

FY 1990
$0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Virginia Polytechnic Institute and State University (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-SA946C) Contacts: K. L. Reifsnider and W. W. Stinchcomb, (703) 961-5316

The purpose of this project is to develop a test system and test methods to obtain information on the properties and performance of ceramic composite materials. The work involves a comprehensive mechanical characterization of composite engineering components such as tubes, plates, shells, and beams subjected to static and cyclic multiaxial loading at elevated temperatures for extended time periods.

Keywords: Ceramics, Composites, Mechanical Properties, Testing

502. Material Data Base Development for Refractories

FY 1990
$0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Massachusetts Institute of Technology (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc., Subcontract No. 19X-07862C) Contact: Oral Buyukozturk, (617) 253-7186

The objective of this project is to generate and compile experimental data on the thermomechanical behavior of selected high-chromia and high-alumina refractories. The work performed on this project supports the work being done by the Tennessee Center for Research and Development to develop user-friendly and intelligent computer-based software for the prediction of thermomechanical behavior of refractory lining systems.

Keywords: Refractory Liners, Stress Analysis, Strain, Mechanical Behavior

503. Advanced Materials and Electrochemical Processes in High-Temperature Solid Electrolytes — FY 1990 $296,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Pacific Northwest Laboratory (Contract No. DE-AC06-76RL01830) Contact: J. L. Bates, (509) 375-2579/FTS 444-2579

The objective of this research is (1) to identify, develop, and demonstrate advanced materials for use as alternative electrodes and current interconnections in solid oxide fuel cells, and (2) to develop an understanding of the synergistic effects of materials properties, structures, and compositions on electrochemical processes related to high-temperature solid electrolyte use in electrochemical cells.

Keywords: Fuel Cells, Electrochemical, Electrolytes

504. Gas Separations Using Inorganic Membranes — FY 1990 $197,000

DOE Contacts: D. C. Cicero, FTS 923-4826 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: B. Z. Egan, (615) 574-6868/FTS 624-6868

The objective of this project is to explore the applicability of inorganic membranes to separate gases at high temperatures and/or in hostile process environments encountered in fossil energy conversion processes such as coal gasification. The program will seek to apply porous membrane technology developed for uranium enrichment to the separation of gases. The program could lead to the development of processes that would improve the economics of fossil energy conversion processes by significantly reducing gas cleanup and separation costs.

Keywords: Membrane, Gas Separation

505. Ceramic Fiber-Ceramic Matrix Hot-Gas Filters — FY 1990 $197,000

DOE Contacts: N. Holcombe, FTS 923-4829 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: D. P. Stinton, (615) 574-4556/FTS 624-4556

This task will develop ceramic fiber-ceramic matrix materials and fabrication techniques suitable for production of hot-gas cleanup filters. The technology developed will be transferred to industry via a research subcontract with an industrial organization (see project described above for the Fabrication of Commercial-Scale Fiber-Reinforced Hot-Gas Filters by Chemical Vapor Deposition) for the production of full-size candle filters.

Keywords: Ceramic Composites, Filters

506. Identification of Materials for Hot-Gas Filter Tubesheets FY 1990 $133,000

DOE Contacts: V. Kothari, FTS 923-4505 and E. E. Hoffman, (615) 576-0735/ FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.) Contact: R. W. Swindeman, (615) 574-5108/FTS 624-5108

The objectives of this work are: (1) to assess current tubesheet designs and blowback manifold materials for ceramic crossflow and ceramic candle filter; (2) to investigate alternative tubesheet designs; (3) to define the strength requirements for ceramic filter tubesheets in hot-gas cleanup systems based on design methodology developed at the Oak Ridge National Laboratory; (4) to collect and analyze data on commercial materials; (5) to collect and analyze data on advanced materials; and (6) to fabricate subsized components (tubesheets) out of the selected materials and characterize its mechanical properties across the thickness and carious orientations. This task is anticipated to result in the recommendation of a tubesheet materials for long-term operation in a high-efficiency hot-gas filter system.

Keywords: Filters, Tubesheets, Alloys

Instrumentation and Facilities

507. Management of the Fossil Energy AR&TD Materials Program FY 1990 $396,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: R. R. Judkins, (615) 574-4572/FTS 624-4572

The overall objective of the Fossil Energy Advanced Research and Technology Development (AR&TD) Materials Program is to conduct a fundamental, long-range research and development program that addresses, in a generic way, the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to manage the Fossil Energy AR&TD Materials Program in accordance with procedures described in the Program Management Plan approved by DOE. This task is responsible for preparing the technical program implementation plan for DOE approval; submitting budget proposals for the program; recommending work to be accomplished by subcontractors and by Oak Ridge National Laboratory (ORNL); placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; and for reporting the progress of the program.

Keywords: Management, Materials Program

508. Materials Specialist Assignment — FY 1990 $69,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contacts: R. R. Judkins, (615) 574-4572/FTS 624-4572

This task involves the assignment of a materials specialist to DOE Fossil Energy to serve as a liaison between the Office of Technical Coordination and the AR&TD Materials Program Offices in Oak Ridge, Tennessee.

Keywords: Management, Materials Program

509. Coal Conversion and Utilization Plant Support Services — FY 1990 $49,000

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (Contract No. DE-AC05-84OR21400, Martin Marietta Energy Systems, Inc.) Contact: J. R. Keiser, (615) 574-4453/FTS 624-4453

The objective of this task is to provide support to the staffs of the DOE Energy Technology Centers and of operating coal conversion and utilization facilities in the areas of materials testing, evaluation, selection, and failure analysis.

Keywords: Testing, Failure Analysis

510. Assessment of Fossil Energy Materials Research Needs — FY 1990 $0 (PF)

DOE Contacts: J. P. Carr, (301) 353-6519/FTS 233-6519 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
National Institute of Standards and Technology (Contract No. DE-A105-89OR21857) Contact: S. J. Dapkunas, (301) 975-6119

The purpose of this activity is to identify long-range materials research and development needs and opportunities as they impact evolving fossil energy technologies. The needs and opportunities that are identified shall be appropriate for future research on the Fossil Energy Advanced Research & Technology Development (AR&TD) Materials Program.

Keywords: Materials, Assessment, R&D Needs

Office of Coal Technology

The Office of Coal Technology is responsible for management of cooperative agreements with industry to foster clean coal technology; for the conduct of research and development programs for coal combustion and conversion, embodying retrofit or near-or mid-term applications such as fluidized-bed combustion and surface coal gasification; and for environmental, health and safety technology integral to such coal combustion and conversion systems.

Division of Clean Coal Technology

Instrumentation and Facilities

511. Materials Technical Support for the Clean Coal Program FY 1990
$0 (PF)

DOE Contacts: R. Santore, FTS 723-6131 and E. E. Hoffman, (615) 576-0735/FTS 626-0735
Oak Ridge National Laboratory (DE-AC05-88OR21400, Martin Marietta Energy Systems, Inc.)
R. R. Judkins, (615) 574-4572/FTS 624-4572 Contact: J. R. Keiser, (615) 574-4453/FTS 624-4453

This task is to provide materials technical support services to the projects on the Clean Coal Program which are being managed by the DOE Pittsburgh Energy Technology Center (PETC). The scope of the work includes assistance to PETC and the Clean Coal Program contractors on any technical issues related to materials performance on their projects. High-risk (in terms of materials degradation) areas will be identified to permit review and study that will minimize failures and thus protect U.S. Government interests in regard to schedules and costs. Emphasis of the project will be placed on prevention, rather than correction, of materials problems. Participation in project and design reviews will be a primary method used to assure that materials problems are avoided. Activities will also include technical consultation, materials testing, recommendations of materials, and failure analyses.

Keywords: Materials, Technical Support

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