DOE/SC-0088

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 2003

October 18, 2004

Annual Technical Report

U.S. Department of Energy
Office of Science
Office of Basic Energy Sciences
Division of Materials Sciences and Engineering
Washington, DC 20585-1290

TABLE OF CONTENTS

Page

Introduction . . . 1
Energy Materials Coordinating Committee Membership List . . . 5
Organization of the Report . . . 8
FY 2003 Budget Summary of DOE Materials Activities . . . 9
Distribution of Funds by Office . . . 11

PROGRAM DESCRIPTIONS

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY . . . 12

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS . . . 13

FREEDOMCAR & VEHICLE TECHNOLOGIES PROGRAM . . . 17
- Materials Technologies Program . . . 19
  - Automotive Propulsion Materials . . . 19
  - Automotive Lightweight Vehicle Materials . . . 22
  - Heavy Vehicle Propulsion System Materials . . . 25
  - High Strength Weight Reduction Materials . . . 33
  - High Temperature Materials Laboratory . . . 35

GEOTHERMAL TECHNOLOGIES PROGRAM . . . 36
- Geothermal Materials . . . 37

HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM . . . 38
- Hydrogen Storage Materials Program . . . 39
- Fuel Cell Materials Program . . . 40

INDUSTRIAL TECHNOLOGIES PROGRAM . . . 43
- Aluminum Subprogram . . . 47
- Glass Subprogram . . . 55
- Metal Casting Subprogram . . . 56
- Steel Subprogram . . . 58
- Materials Subprogram . . . 62

SOLAR ENERGY TECHNOLOGY PROGRAM . . . 71
- National Photovoltaics Program . . . 72

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM . . . 75
- Financial Assistance Program . . . 77
  - Inventions & Innovation (I&I) . . . 77
  - National Industrial Competitiveness Through Energy, Environment and Economics ($NICE^3$) . . . 84

TABLE OF CONTENTS (continued)

Page

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION 87
High Temperature Superconductivity for Electric Systems 88

OFFICE OF SCIENCE 93
Office of Basic Energy Sciences 103
Division of Materials Sciences and Engineering 103
Division of Scientific User Facilities 106
Office of Advanced Scientific Computing Research 106
Technology Research Division 106
Laboratory Technology Research Program 106
Small Business Innovation Research Program 108
Small Business Technology Transfer Research Program 118
Office of Fusion Energy Sciences 119
Office of Biological & Environmental Research 121

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY 127
Office of Space and Defense Power Systems 128
Space and National Security Programs 128
Office of Advanced Nuclear Research . . . . .
Advanced Fuel Cycle Initiative 129
Nuclear Hydrogen Initiative 130

NATIONAL NUCLEAR SECURITY ADMINISTRATION 132
Office of Naval Reactors 134
Office of Defense Programs 134
The Weapons Research, Development and Test Program 134
Sandia National Laboratories 134
Lawrence Livermore National Laboratory 149

OFFICE OF FOSSIL ENERGY 152
Office of Advanced Research 154
Advanced Research Materials Program 154
Ultra-Supercritical Steam and Power Plant Research 164
Advanced Metallurgical Processes Program 164

DIRECTORY 167

INDEX 187

LIST OF TABLES

Table 1 Energy Materials Coordinating Committee Membership List 5
Table 2 Distribution of Funds by Office 11

INTRODUCTION

The DOE Energy Materials Coordinating Committee (EMaCC) serves primarily to enhance coordination among the Department's materials programs and to further effective use of materials expertise within the Department. These functions are accomplished through the exchange of budgetary and planning information among program managers and through technical meetings/workshops on selected topics involving both DOE and major contractors. In addition, EMaCC assists in obtaining materials-related inputs for both intra- and interagency compilations.

Topical subcommittees of the EMaCC are responsible for conducting seminars and otherwise facilitating information flow between DOE organizational units in materials areas of particular importance to the Department. The EMaCC Terms of Reference were recently modified and developed into a Charter that was approved on June 5, 2003. As a result of this reorganization, the existing subcommittees were disbanded and new subcommittees are being formed.

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 pages 5-7.

Four meetings were scheduled for 2003-2004. The dates and minutes from the meetings are as follows:

ENERGY MATERIALS COORDINATING COMMITTEE

MINUTES, MEETING OF OCTOBER 16, 2003

The EMaCC meeting was held in room E-301 Germantown building on Thursday, October 16, 2003. The meeting started at 10:15 A.M. and ended at 11:30 A.M. The chairman, Dr. Dale Koelling, opened the meeting by having the participants introduce themselves.

Kristin Bennett (BES) described the five nano-centers being created. Send your browser to http://www.science.doe.gov/bes/ NNI.htm or http://www.science.doe.gov/bes/User_Facilities/dsuf/nanocenters.htm to find the links for each of these five centers. Although there is the temptation to get off into the technical details, the essential points for EMaCC are:

- The nanocenters are user facilities. The simplest way to emphasize this is that researchers can apply for time on the resources of these centers. It will be allocated by user committees and will be no cost (except for proprietary efforts).
- The ground is, or shortly will be, being broken for the buildings to house these centers for completion in 2005 or 2006.
- However, some resources are already available now under the JUMPSTART program.

D. Koelling and J. Zhu reported on a meeting they attended at the National Academy of Sciences on September 29, 2003, where the possible formation of a Materials Roundtable was discussed. What is envisioned is a multi-layered grouping that would provide coordination and communication amongst all sectors involved with materials. The next step envisioned is a broader meeting to occur on December 11, 2003 (tentative date). An list of attendees and the two page description handed out at the meeting were provided to those attending the EMaCC meeting. Anyone else interested can request a copy from Koelling or Zhu.

The minutes of the meeting held on July 15, 2003, were approved. Tom Kiess agreed to serve as chair of the new subcommittee forming with interest in materials in a radiation environment (committee name still to be chosen). The slate of nominees for FY04 EMaCC officers was then presented and further nominations solicited. Being no further nominations, it was moved that the officers be elected unanimously and the motion carried. Accordingly, the officers for 2003 are Lane Wilson, chair, and Jane Zhu, executive secretary.

The date of the next meeting was not discussed (time constraints). Following the usual scheme, the initial target date should be in January 2004. The meeting will occur in Forrestal.

CALENDAR ITEMS

Oct. 20-21, 2003: Basic Energy Sciences Advisory Committee meeting, Rockville, MD (minutes and Presentations as well as future meetings can be found through the hyperlink). Contact: Sharon Long.

Oct. 30, 2003: Interagency Metals Research Coordination Group, 530, NSF. Contact: S. Dillich

Nov. 4-5, 2003:	Interagency NDE Coordination Group. Suite 509, 1815 N. Fort Myer Drive. Contact: T. Fitzsimmons
Nov. 13-14, 2003:	Solid State Lighting Workshop,. Doubletree Inn, Crystal City, VA. Contact: J.R. Brodrick
Nov. 19-20, 2003:	Metals and Engineering Physics (MEP) Sandia-Albuquerque. External Peer Review, Sandia Labs, Albuquerque, NM. Contact: Y. Chen
Nov. 24-25, 2003:	Condensed Matter Physics & Materials Chemistry (CMPMC) External Peer Review - primarily Materials Chemistry, Oak Ridge National Laboratory, ORNL. Contact: R. Kelley
Dec. 1-5, 2003:	Materials Research Society meeting, Boston. Contact: R. Gottschall
Dec. 9-11, 2003:	(CMPMC) External Peer Review - primarily Condensed Matter Physics, Oak Ridge National Laboratory, ORNL. Contact: J. Horwitz
Dec. 15-16, 2003:	Council on Materials Sciences and Engineering, Gaithersburg Marriott Washingtonian Center. Contact: Christie Ashton
Jan. 14-16, 2004:	MEP Lawrence Berkeley Lab. External peer review, LBNL. Contact A. Carim
Mar. 1-2, 2004:	CMPMC External Peer Review at Los Alamos National Laboratory, LANL. Contact: J. Horwitz
Mar. 3-4, 2004:	CMPMC External Peer Review at Sandia National Laboratory, Albuquerque. Contact: J. Horwitz

Note: Observers are welcome at the external peer reviews.

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JANUARY 22, 2004, FORRESTAL BUILDING

The EMaCC meeting was held in room GH035 Forrestal building on Thursday, January 22, 2003.The meeting started at 10:15 A.M. and ended at 11:30 A.M. The chairman, Dr. Lane Wilson, opened the meeting with participants introducing themselves, and led discussions about the EMaCC charter, future meetings and the annual reports.

Robert Gottschall (BES) reported on a workshop, Corrosion Issues of Relevance to the Yucca Mountain Waste Repository, which was jointly sponsored by the Office of Basic Energy Sciences and the Office of Civilian Radioactive Waste Management (OCRWM). The workshop was held in Bethesda, MD on July 29 and 30th 2003, and organized by Prof. Joe H. Payer of Case Western Reserve University and Professor John R. Scully of University of Virginia. The topics covered by the workshop included localized corrosion: pitting and crevice corrosion, stress corrosion cracking/hydrogen damage, long term passivity, life prediction and damage evolution (performance), environment on metal surfaces and in occluded sites, alloy stability and aging, fabrication and advanced materials, and advanced research tools and techniques. More details about the workshop are available at the website http://www.virginia.edu/cese/doe/DoEworkshop.html.

Sue Lesica (NE) reported on the activities of the Fission-Fusion Subcommittee of EMaCC and the Materials Research in Nuclear Energy. She showed highlights ('03) and future plans ('04) on areas such as mechanical testing and microstructure, data in a Materials Handbook, and atomistic modeling of He in body-centered cubic Fe. Further information about programs in the Office of Nuclear Energy, Science and Technology can be found on the web at www.nuclear.gov.

The minutes of the meeting held on October 16, 2003, were approved.

Lane Wilson continued to lead the discussion on the issues raised earlier in the meeting, and asked for input from all interested for suggestions on future meeting agendas, recommendations for speakers, and the format of the EMaCC annual reports. He asked the committee to consider if any other subcommittees are desired, such as a hydrogen group. Rich Silberglitt has been facilitating the publication of the EMaCC annual reports. Silberglitt explained how the input for the reports was collected.

The next EMaCC meeting will occur in Germantown (following our tradition in alternating the meeting places) on Thursday April 22, 2004.

CALENDAR ITEMS

March 4-5, 2004:	Advanced Reactor, Fuel Cycle, and Energy Products Workshop for Universities, Gaithersburg, MD. Contact: Sue Lesica.
April 14, 2004:	Interagency Coordinating Committee on Structural Ceramics meeting, at the National Science Foundation in Arlington, Virginia. Contact: Jane Zhu.
June 3-4, 2004:	Center of Excellence for the Synthesis and Processing of Advanced Materials meeting, Germantown, MD. Contact: Bob Gottschall.

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APRIL 22, 2004, GERMANTOWN

The EMaCC meeting was held in room E-401 Germantown building on Thursday, April 22, 2004. The meeting started at 10:15 A.M. and ended at 11:40 A.M. The chairman, Dr. Lane Wilson, opened the meeting with participants introducing themselves.

Sam Berk (FES/SC) talked about the controlled thermonuclear fusion in deuterium-tritium plasmas as an energy source, science issues in the magnetic confinement of plasmas and fusion experiments by the tokamak. The fusion power plant concept is based on conventional means of electricity generation. Dr. Berk also talked about the fusion power core, the ARIES-AT blanket concept, and the requirements for blanket materials.

Steve Zinkle (ORNL) gave a talk on Overview of Fusion Structural Materials Research. The topics reviewed included: the research scope of fusion materials sciences program; the fundamental studies of radiation-induced defects and their effects on material properties, such as multiscale modeling, radiation-induced defect production and accumulation, and mechanical deformation and fracture mechanisms; and the development of improved structural materials, such as the nanocomposite ferritic steel, refractory alloys, ceramic composites, and Cu alloys. Dr. Zinkle concluded that reduced activation materials with properties comparable or superior to conventional materials have been developed by the fusion materials community.

Fusion materials R&D efforts have led to the development of materials with good radiation resistance during fission reactor irradiation up to 10-50 dpa (displacement per atom) and higher. The main uncertainty is the microstructural evolution and property degradation that may occur for fusion neutron exposures above ~10 dpa (~100 appm He). A fusion neutron source is needed to develop and qualify structural materials for Demo. The successful development of fusion energy will require a sustained R&D program in materials and other technologies. Currently available materials will serve as stepping stones to future, improved fusion materials.

The minutes of the meeting held on January 22, 2004, were approved. Lane Wilson led the discussion session and suggested to form an EMaCC subcommittee on hydrogen. Further discussion on this topic is encouraged among EMaCC members.

CALENDAR ITEMS

June 21-24, 2004: Annual review of the DOE-EERE Industrial Technologies Program: Materials, Glass, and Sensors and Automation portfolios and projects, Gateway Marriott in Arlington, Virginia. Contact: Sara Dillich

June 23-24, 2004: DOE NanoSummit: Nanoscale Science and Our Energy Future will be held at the Wardman Park Marriott in Washington, D.C. Registration is free to DOE employees, https://public.ornl.gov/conf/nanosummit2004/registration.cfm.

August 26, 2004: Basic Energy Sciences Advisory Committee Meeting, Doubletree Hotel, Rockville, MD. Contact: Karen Talamini

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Alan Hartman	ARC	Hartman@alrc.doe.gov (via Web conference)

JULY 20, 2004, GERMANTOWN

The EMaCC meeting was held in room E-301 Germantown building on Tuesday, July 20, 2004. Minutes of this meeting will be published, after approval, in the next EMaCC Report.

The EMaCC reports to the Director of the Office of Science in his or her capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC Charter. This report summarizes EMaCC activities for FY 2003 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 2003 was Dr. Dale Koelling. The compilation of this report was performed by Dr. Jane Zhu, EMaCC Executive Secretary for FY 2004, with the assistance of the RAND Corporation. Financial support was provided by the Industrial Materials for the Future program of the Industrial Technologies Program and by the Office of Basic Energy Sciences.

Dr. Lane Wilson
National Energy Technology Laboratory
EMaCC Chair, FY 2004

TABLE 1
ENERGY MATERIALS COORDINATING COMMITTEE MEMBERSHIP LIST

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technologies	Marc Lafrance, EE-2J	202-586-9142
FreedomCAR & Vehicle Technologies		
Automotive Lightweight Vehicle Materials	Joseph Carpenter, EE-2G	202-586-1022
Heavy Vehicle Materials Technologies	Sidney Diamond, EE-2G	202-586-8032
Geothermal Technologies		
Geothermal Materials	Raymond LaSala, EE-2C	202-586-4198
Hydrogen, Fuel Cells & Infrastructure Technologies		
Fuel Cell Materials	Nancy Garland, EE-2H JoAnn Milliken, EE-2H	202-586-5673 202-586-2480
Industrial Technologies		
Materials and Materials Processes	Sara Dillich, EE-2F	202-586-7925
Materials Liaison	Charlie Sorrell, EE-2F	202-586-1514
Solar Energy Technology		
National Photovoltaic Program	Richard King, EE-2A Ray Sutula, EE-2A	202-586-1693 202-586-8064
ELECTRIC TRANSMISSION AND DISTRIBUTION		
High Temperature Superconductivity	James Daley, TD-2	202-586-1165

ORGANIZATION	REPRESENTATIVE	PHONE NO.
SCIENCE		
Basic Energy Sciences		
Materials Sciences and Engineering	Pat Dehmer, SC-10	301-903-3081
Materials and Engineering Physics	Robert J. Gottschall, SC-13	301-903-3978
	Altaf Carim, SC-13	301-903-4895
	Yok Chen, SC-13	301-903-4174
	Tim Fitzsimmons, SC-13	301-903-9830
	Jane Zhu, SC-13	301-903-3811
Condensed Matter Physics and Materials Chemistry	W. Oosterhuis, SC-13	301-903-4173
	Richard Kelly, SC-13	301-903-6051
	Helen Kerch, SC-13	301-903-2346
	Arivinda M. Kini, SC-13	301-903-3565
	Dale Koelling, SC-13	301-903-2187
	Matesh (Mat) Varma, SC-13	301-903-3209
Chemical Sciences, Geosciences and Biosciences	Nick Woodward, SC-14	301-903-4061
Advanced Scientific Computing Research		
Technology Research	Samuel J. Barish, SC-32	301-903-2917
Fusion Energy Sciences		
Facilities and Enabling Technologies	Sam Berk, SC-52	301-903-4171
Biological and Environmental Research		
Medical Sciences	Larry James, SC-73	301-903-7481
ENVIRONMENTAL RESTORATION AND WASTE MANAGEMENT		
Integration and Disposition		
Technical Program Integration	Doug Tonkay, EM-22	301-903-7212
Science and Technology		
Basic and Applied Research	Chet Miller, EM-52	202-586-3952

ORGANIZATION	REPRESENTATIVE	PHONE NO.
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Advanced Nuclear Research	Susan Lesica, NE-20	301-903-8755
Nuclear Facilities Management	John Warren, NE-40 Bob Lange, NE-40	301-903-6491 301-903-2915
Space and Defense Power Systems	John Dowicki, NE-50	301-903-7729
NATIONAL NUCLEAR SECURITY ADMINISTRATION		
Naval Reactors	David I. Curtis, NR-1	202-781-6141
Defense Programs		
Defense Science	Bharat Agrawal, NA-113-2	301-903-2057
CIVILIAN RADIOACTIVE WASTE MANAGEMENT		
Waste Acceptance and Transportation	Thomas Kiess, RW-40E	202-586-5679
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser, FE-25	301-903-2786

ORGANIZATION OF THE REPORT

The FY 2003 budget summary for DOE Materials Activities is presented on pages 9 and 10. The distribution of these funds between DOE laboratories, private industry, academia and other organizations is presented in tabular form on page 11.

Following the budget summary is a set of detailed program descriptions for the FY 2003 DOE Materials activities. These descriptions are presented according to the organizational structure of the Department. A mission statement, a budget summary listing the project titles and FY 2003 funding, and detailed project summaries are presented for each Assistant Secretary office, the Office of Science, and the National Nuclear Security Administration. The project summaries also provide DOE, laboratory, academic and industrial contacts for each project, as appropriate.

FY 2003 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES

These budget numbers represent materials-related activities only. They do not include those portions of program budgets which are not materials related.

	FY 2003
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$2,143,000
FREEDOMCAR & VEHICLE TECHNOLOGIES PROGRAM	$36,978,000
Materials Technologies Program	36,978,000
Automotive Propulsion Materials	1,850,000
Automotive Lightweight Vehicle Materials	15,515,000
Heavy Vehicle Propulsion System Materials	4,987,000
High Strength Weight Reduction Materials	9,026,000
High Temperature Materials Laboratory	5,600,000
GEOTHERMAL TECHNOLOGIES PROGRAM	$310,000
Geothermal Materials	310,000
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM	$6,527,500
Hydrogen Storage Materials Program	5,535,000
Fuel Cell Materials Program	992,500
INDUSTRIAL TECHNOLOGIES PROGRAM	$22,834,600
Aluminum Subprogram	5,951,600
Glass Subprogram	200,000
Metal Casting Subprogram	1,279,000
Steel Subprogram	3,468,000[1]
Materials Subprogram	11,936,000
SOLAR ENERGY TECHNOLOGY PROGRAM	$26,623,000
National Photovoltaics Program	26,623,000
WEATHERIZATION & INTERGOVERNMENTAL PROGRAM	$0[2]
Financial Assistance Program	0
Inventions & Innovation (I&I)	0
National Industrial Competitiveness Through Energy, Environment and Economics (NICE[3])	0
OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION	$38,010,000
High Temperature Superconductivity for Electric Systems	38,010,000

[1]For every project within the American Iron and Steel Institute's (AISIs) Technology Roadmap Program (TRP), the funding shown is the total over the life of the project. Total DOE/ITP TRP funding in FY03 was $3,468,000.

[2]Prior year funding

FY 2003 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES (continued)

	FY 2003
OFFICE OF SCIENCE	$607,694,828
Office of Basic Energy Sciences	550,604,000
Division of Materials Sciences and Engineering	233,940,000
Division of Scientific User Facilities	316,664,000
Office of Advanced Scientific Computing Research	45,870,828
Technology Research Division	45,870,828
Laboratory Technology Research Program	749,000
Small Business Innovation Research Program	42,060,212
Small Business Technology Transfer Research Program	3,061,616
Office of Fusion Energy Sciences	9,000,000
Office of Biological & Environmental Research	2,220,000
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$9,476,000
Office of Space and Defense Power Systems	6,466,000
Space and National Security Programs	6,466,000
Office of Advanced Nuclear Research	3,010,000
Advanced Fuel Cycle Initiative	2,260,000
Nuclear Hydrogen Initiative	750,000
NATIONAL NUCLEAR SECURITY ADMINISTRATION	$112,368,000
Office of Naval Reactors	83,400,000[3]
Office of Defense Programs	28,968,000
The Weapons Research, Development and Test Program	28,968,000
Sandia National Laboratories	17,535,000
Lawrence Livermore National Laboratory	11,433,000
OFFICE OF FOSSIL ENERGY	$12,020,000
Office of Advanced Research	12,020,000
Advanced Research Materials Program	6,049,000
Ultra-Supercritical Steam and Power Plant Research	1,570,000
Advanced Metallurgical Processes Program	4,401,000
TOTAL	$874,984,928

[3]This excludes $52.8 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

The distribution of these funds between DOE laboratories, private industry, academia and other organizations is listed below.

TABLE 2
DISTRIBUTION OF FUNDS BY OFFICE

Office	DOE Laboratories	Private Industry	Academia	Other	Total
Building Technologies Program	$1,165,000	$811,000	$167,000	$0	$2,143,000
FreedomCAR & Vehicle Technologies	$23,269,000	$10,460,000	$1,969,000	$1,280,000	$36,978,000
Geothermal Technologies Program	$310,000	$0	$0	$0	$310,000
Hydrogen, Fuel Cells and Infrastructure Technologies Program	$5,017,500	$1,250,000	$260,000	$0	$6,527,500
Industrial Technologies Program	$6,700,692	$9,222,744	$5,572,516	$1,338,648	$22,834,600[4]
Solar Energy Technology Program	$26,623,000	$0	$0	$0	$26,623,000
Weatherization & Intergovernmental Program	$0	$0	$0	$0	$0[5]
Office of Electric Transmission and Distribution	$25,000,000	$11,500,000	$1,000,000	$510,000	$38,010,000
Office of Science	$386,144,000	$45,121,828	$176,429,000	$0	$607,694,828
Office of Nuclear Energy, Science and Technology	$8,726,000	$0	$750,000	$0	$9,476,000
National Nuclear Security Administration	$112,368,000	$0	$0	$0	$112,368,000[6]
Office of Fossil Energy	$10,786,000	$385,000	$849,000	$0	$12,020,000
TOTALS	**$606,109,192**	**$78,750,572**	**$186,996,516**	**$3,128,648**	**$874,984,928**

[4]For every project within the American Iron and Steel Institute's (AISIs) Technology Roadmap Program (TRP), the funding shown is the total over the life of the project. Total DOE/ITP TRP funding in FY03 was $3,468,000.

[5]Prior year funding

[6]This excludes $52.8 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

The Office of Energy Efficiency and Renewable Energy (EERE) mission is to strengthen America's energy security, environmental quality and economic vitality in public-private partnerships that:

Enhance energy efficiency and productivity
Bring clean, reliable and affordable energy technologies to the marketplace
Make a difference in the everyday lives of Americans by enhancing their energy choices and their quality of life

EERE's program activities are conducted in partnership with the private sector, state and local government, DOE national laboratories, and universities. In July 2002, EERE reorganized to strengthen its focus on programs and these partnerships.

In contrast to the previous organization into five energy sectors—industry, transportation, buildings, power and Federal agencies—EERE is now organized around eleven energy programs:

Biomass Program
Building Technologies Program
Distributed Energy & Electricity Reliability Program
Federal Energy Management Program
FreedomCAR & Vehicle Technologies Program
Geothermal Technologies Program
Hydrogen, Fuel Cells & Infrastructure Technologies Program
Industrial Technologies Program
Solar Energy Technology Program
Weatherization & Intergovernmental Program
Wind & Hydropower Technologies Program

Several of these programs sponsor materials research and the breadth of the EERE materials research is substantial, including research on metals, ceramics, polymers, magnetic materials, superconductors, composites, coatings, nanoscale materials, advanced forming, welding and joining, corrosion, erosion, wear and other areas.

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 2003
OFFICE OF BUILDING TECHNOLOGIES - GRAND TOTAL	$2,143,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$717,000
Non-HCFC Closed-Cell Foam Insulation	50,000
Hygrothermal Material Property Measurements & Modeling Upgrades and Applications	500,000
Floor Tile with Phase Change Materials	167,000
FENESTRATION MATERIALS DEVELOPMENT	$1,426,000
Development of Electrochromic Materials and Coatings	1,103,000
Development of Aerogel Materials for R10/ inch Transparent Window Insulation	323,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING RESEARCH AND STANDARDS

PROGRAM GOALS

The goal of the program is to develop advanced windows, new building materials and building envelope systems that can contribute to the DOE energy efficiency goal of constructing zero energy buildings. These activities will result in building systems that consume significantly less energy while drastically reducing peak electricity demand.

PROGRAM OBJECTIVES

The program objectives are:

1) Development of Advanced Windows that have highly insulating properties, that offer dynamic solar heat gain control, and have very low solar heat gain coefficients
2) Develop moisture design guidelines for all regions of the country using fundamental material properties and advanced modeling to ensure that building envelope performance can be increased without moisture and mold problems
3) Develop the scientific and engineering tools for development, demonstration and production of more energy efficient, durable affordable and sustainable building envelope system technologies
4) Identify and develop new or improved insulation and other building materials
5) Develop and standardize laboratory methods for characterizing new and existing materials
6) Make recommendations on the effective use of building materials
7) Develop a fundamental understanding of the physics of heat, air, and moisture flow in advanced and conventional building materials
8) Develop and standardize field and laboratory whole envelope system performance test protocols to stimulate development and investment in energy efficient envelope technologies
9) Provide data developed for energy efficient building envelope and material technologies for inclusion into the Building Codes and Standards

The DOE contact is Marc LaFrance (202) 586-9142

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

1. **NON-HCFC CLOSED-CELL FOAM INSULATION**
   $50,000
   DOE Contact: Marc LaFrance (202) 586-9142
   ORNL Contact: Ken Wilkes (865) 574-5931

This project is for the development of foam insulations that use alternative blowing agents as drop-in replacements for the CFC blowing agents that were previously used in the manufacture of foam insulation products and for the HCFC blowing agents that are currently being used. Prototype foam insulation boards and refrigerator panels were sent to ORNL for testing and evaluation. Long-term tests are being conducted to determine thermal properties and aging characteristics. Models are being developed for aging processes, including the effects of facing materials.

Keywords: CFC, Foam Insulation, Insulation Sheathing, Roofs, HCFC, Refrigerators

2. **HYGROTHERMAL PROPERTY MEASUREMENTS & MODELING UPGRADES AND APPLICATIONS**
   $500,000
   DOE Contact: Marc LaFrance (202) 586-9142
   ORNL Contact: Andre Desjarlais (865) 574-0022

The objective of this task is to measure the hygrothermal properties of a broad range of building materials that are required for modeling of moisture transport in building envelopes. Such property values are needed as inputs to moisture simulation models and provide the link between the models and large-scale experiments on moisture transfer in building envelope components. The intent of the proposed work is to develop unique hygrothermal-durability modeling capability to permit prediction long-term performance of wall systeMs. The model, WUFI, is a joint project with Germany. The model can be downloaded for free in North Amercia at http://www.ornl.gov/ORNL/BTC/moisture/index.html. The model will be used to develop guidelines for moisture management strategies for wall systems to meet user requirements of long-term performance and durability for the wide range of climate zones across North America. Properties that will be measured include sorption and suction isotherms, vapor permeance, liquid diffusivity, air permeability, specific heat, and thermal conductivity.

Where applicable, the properties will be measured as functions of moisture content and temperature. The laboratory will support other research on measurements and modeling of coupled heat, air, and moisture transfer in building envelopes.

Keywords: Hygrothermal, Moisture, Building Materials, Heat-Air-Moisture, Properties

3. **PHASE CHANGE MATERIALS IN FLOOR TILES FOR THERMAL STORAGE**
DOE $167,000, Colorado State Univ. $42,000
DOE Contact: Marc LaFrance (202) 586-9142
CSU Contact: Doug Hittle (970) 229-9403

Colorado State University received a competitively awarded project to develop a floor tile with phase change material incorporated into the bonding resins. The goal is to develop a tile that can act as a thermal storage device that will retain passively gained heat until later in the evening when the stored heat can be used to offset the heating requirements. Initial prototypes have been developed. The next key step will be to attract a manufacturing partner.

Keywords: Thermal Storage, Phase Change, Tiles, Passive Heating

FENESTRATION MATERIALS DEVELOPMENT

4. **DEVELOPMENT OF “ELECTROCHROMIC” MATERIALS AND COATINGS**
DOE Contact: Marc LaFrance (202) 586-9142

DOE has been working on a variety of “electrochromic” research projects to develop glazings that can control the visual transmittance and solar heat gain for windows. Once commercialized, dynamic windows will significantly reduce energy consumption and will reduce peak energy demand.

DOE $488,000, Sage $140,000
SAGE Electrochromic Inc.: Neil Sbar (507) 333-0078

Through competitively awarded contracts that include manufacturer cost share, Sage is developing a “ceramic” based electrochromic device. Fundamental material science and deposition processes are being developed to allow for uniform, reliable, durable and cost effective devices that have a wide range of dynamic control. Currently, Sage is at the pilot production phase, although material enhancements and yield improvements continue to be investigated. Samples have performed very well through extended durability testing.

$465,000
LBNL: Steve Selkowitz (510) 486-5064

The recent discovery of metal hydride and non-hydride switchable mirrors that can be modulated from highly reflecting (metallic) to highly absorbing (black) to highly transparent (semiconducting) could be the basis for a much simpler, less expensive device. Like tungsten oxide, the reflective metal hydrides can be used in either a solid-state or “gasochromic” configuration. The hydrides lend themselves particularly well to the gasochromic device which might require only the deposition of a thin metal coating at high rate in a standard industrial sputter system (avoiding the need for thick, costly transparent conducting and electrolyte layers). Lithium-based reflective electrochromic devices can use the same electrolytes and counter electrodes currently used for absorbing devices. Like tungsten oxide, the active layer is transparent when reduced. Modulation of infrared transmittance and reflectance is enhanced by the absence of a transparent conductor.

Current tasks are to develop and further characterize the class of variable reflectance electrochromic coatings. Explore alternative metals and replacement of hydrogen-based devices with lithium based electrochemistry. Issues that need to be addressed are morphological changes during cycling, alloying for stability and improved reflectivity, electrolyte interactions, and intralayer conductivity. Characterize spectral optical properties across complete dynamic switching range. Continue investigation of degradation mechanisms in metal hydride systems and develop mitigation strategies. Pursue development of prototype devices using both solid state and gasochromic structures in collaboration with industrial partners.

$150,000
LANL: Anthony Burrell (505) 667-9342

LANL has demonstrated that ionic liquids are effective components in electrochromic technologies. Chemical and material analyses will be conducted to establish an ionic liquid with dyes that are stable in the presence of Ultra Violet light. Similar electrochromic devices have been commercialized for rear view mirrors, but these are highly unstable in the presence of UV which is needed for the window market. Initial prototypes have been developed with a large dynamic range of solar heat control and have tested well at high and low temperatures. After UV stability has been established, the next key milestone will be to conduct full scale durability tests, along with the development of polymer based fluid properties.

Keywords: Electrochromic, Dynamic Windows, Solar Heat Gain Coefficient, Solar Control, Ionic Fluids, Gasochromic

5. **DEVELOPMENT OF TRANSPARENT AEROGELS R10/INCH FOR WINDOWS**
DOE $323,000, Aspen Aerogels $81,000
DOE Contact: Marc LaFrance (202) 586-9142
Aspen Aerogels, Inc.: George Gould
(508) 481-5058

Aspen Aerogels has developed non-transparent aerogels for a range of product applications that have been commercialized. However, this competitively awarded research is focused on the development of highly transparent sheet material that can be used in the space gap of windows with a thermal resistance of R10 per inch. Technical challenges include the consistent and reliable production of highly transparent samples that offer improved structural integrity with high levels of visual clarity. Activities include development of fundamental precursor chemical compositions, along with production development techniques to reduce manufacturing costs.

Keywords: Aerogels, Advanced Insulation

FREEDOMCAR & VEHICLE TECHNOLOGIES

	FY 2003
FREEDOMCAR & VEHICLE TECHNOLOGIES - GRAND TOTAL	$36,978,000
MATERIALS TECHNOLOGIES PROGRAM	$36,978,000
AUTOMOTIVE PROPULSION MATERIALS	$1,850,000
Technical Project Management	150,000
Low-Cost, High Energy Product Permanent Magnets	300,000
Characterization of Permanent Magnets	50,000
Carbon Foam for Electronics Cooling	300,000
Mechanical Reliability of Electronic Materials and Electronic Devices	100,000
Microwave-Regenerated Diesel Engine Exhaust Particulate Filter Technology	200,000
Material Support for Nonthermal Plasma Diesel Engine Exhaust Emission Control	100,000
Fabrication of Small Injector Orifices	180,000
Technology for Producing Small Holes in Advanced Materials	100,000
Electrochemical No_x Sensor for Monitoring Diesel Emissions	370,000
AUTOMOTIVE LIGHTWEIGHT VEHICLE MATERIALS	$15,515,000
Low-cost High Performance Wrought Aluminum Components for Automotive Applications	360,000
Low-cost High Performance Cast Light Metals for Automotiveapplications	450,000
Advanced Materials and Processes for Automotive Applications	475,000
Technology Assessment and Evaluation	1,915,000
Advanced Joining Technologies	1,350,000
High Strain Rate Deformation of Materials	1,050,000
Reinforced Composite Materials, Durability, and Enabling Technologies	750,000
USAMP Cooperative Agreement	4,450,000
Development of Low-cost Carbon Fiber	1,807,000
Recycling	1,100,000
Structural Reliability of Lightweight Glazing Alternatives	315,000
High Rate Processing Technologies for Polymer Composite Material	1,493,000
HEAVY VEHICLE PROPULSION MATERIALS	$4,987,000
Smart Materials for Fuel System Actuators	400,000
Cost-Effective Smart Materials for Diesel Engine Applications	300,000
Manufacturing Technology for Cermet Components	75,000
Intermetallic-Bonded Cermets	100,000
High-Toughness Materials	300,000
Materials for Exhaust Aftertreatment	400,000
Catalyst Characterization	200,000
Development of No_x Sensors for Heavy Vehicle Applications	200,000
Electron Microscopy for Characterization of Catalyst Microstructures and Deactivation Mechanisms	200,000
Microstructural Changes in No_x Trap Materials under Lean and Rich Conditions at High Temperatures	100,000
Aftertreatment Catalysts Materials Research	85,000
Advanced Materials for Lightweight Valve Train Components	189,000
Engineered Surfaces for Diesel Engine Components	200,000
Cermet Materials for Diesel Engine Wear Applications	125,000
Mechanical Characterization	80,000
NDE of Diesel Engine Components	210,000
Durability of Diesel Engine Component Materials	200,000
Life Prediction of Diesel Engine Components	200,000
Low-Cost Manufacturing of Precision Diesel Engine Components	200,000

FREEDOMCAR & VEHICLE TECHNOLOGIES

	FY 2003
MATERIALS TECHNOLOGIES PROGRAM (continued)	
HEAVY VEHICLE PROPULSION MATERIALS (continued)	
Advanced Machining and Sensor Concept	75,000
Advanced Cast Austenitic Stainless Steels for High-Temperature Exhaust Components	160,000
TiAl Nanolaminate Composites	75,000
Synthesis of Powders for Titanium Carbide/nickel Aluminide Cermets	48,000
Diesel Exhaust Gas Recirculation Corrosion Effects	50,000
Laser Surface Texturing of Lubricated Ceramic Parts	50,000
Low Cost Titanium Feedstock Consolidation Process	100,000
High Density Infrared Surface Treatment of Materials for Heavy-duty Vehicles	70,000
High Temperature Aluminum Alloys	90,000
Rolling Contact Fatigue	200,000
IEA Implementing Agreement for a Programme of Research and Development on Advanced Materials for Transportation Applications	200,000
Testing Standards	105,000
HIGH STRENGTH WEIGHT REDUCTION MATERIALS	$9,026,000
Design, Analysis and Development of Lightweight Frames for Truck and Bus Applications	891,000
Development of Advanced Casting Technologiesmetal Compression Forming (Mcf) for Production of High Integrity Truck Components	715,000
Advanced Forming Technologies for Lightweight Alloys	550,000
Development of Carbon Monliths for Safe, Low Pressure Adsorption Storage and Release Natural Gas	550,000
Improved Materials for Heavy Vehicle Friction and Brake Applications	525,000
High Conductivity Carbon Foams for Thermal Management	125,000
Advanced Joining Technology Development	820,000
Development of Advanced Materials for Heavy Vehicle Applications	975,000
Implementation of Lightweight Materials in Heavy Vehcile Structural Applications	2,175,000
Technology Assessment and Evaluation	1,700,000
HIGH TEMPERATURE MATERIALS LABORATORY	$5,600,000
High Temperature Materials Laboratory User Program	5,600,000

FREEDOMCAR & VEHICLE TECHNOLOGIES PROGRAM

The Office of FreedomCAR and Vehicle Technologies (OFCVT) seeks to develop, in cooperation with industry, advanced technologies that will enable the U.S. transportation sector to be energy efficient, shift to alternative fuels and electricity, and minimize the environmental impacts of transportation energy use. Timely availability of new materials and materials manufacturing technologies is critical for the development and engineering of these advanced transportation technologies. Materials R&D is conducted to address critical needs of automobiles and heavy vehicles. Another important aspect of these activities is the partnership between the Federal government laboratories and U.S. industry, which ensures that the R&D is relevant and that federal research dollars are highly leveraged.

Within OFCVT, the bulk of the materials R&D is carried out through the Materials Technologies program, with additional specialty materials R&D in the Electric Drive Vehicle Technologies program. The Propulsion Materials Technologies program develops: a) Automotive Propulsion Materials to enable advanced propulsion systems for hybrid vehicles, and b) Heavy Vehicle Propulsion System Materials. In collaboration with U.S. industry and universities, efforts in heavy vehicle propulsion system materials focus on the materials technology critical to the development of the low emission, 55 percent efficient (LE-55) heavy-duty and multi-purpose Diesel engines, such as: manufacturing of ceramic and metal components for high-efficiency turbocharger and supercharger; thermal insulation, for reducing engine block cooling, lowering ring-liner friction and reducing wear; high-pressure fuel injection materials; and exhaust after treatment catalysts and particulate traps. The DOE contacts are Nancy Garland (202) 586-5673, for automotive propulsion materials and Sid Diamond (202) 586-8032 for heavy vehicle propulsion materials. The Electric Vehicle R&D program includes the support of Advanced Battery Development for electric and hybrid vehicle applications. The DOE contact is Tien Duong (202) 586-2210.

The Lightweight Materials Technology program focuses on two areas: (a) Automotive Lightweighting Materials to reduce vehicle weight and thereby decrease fuel consumption. The program seeks to develop advanced materials with the required properties and the processes needed to produce them at the costs and volumes needed by the automotive industries. Improved materials for body, chassis, and powertrain are critical to attaining the challenging performance standards for advanced automotive vehicles, and (b) High Strength Weight Reduction Materials. In the area of high strength weight reduction materials, energy savings from commercial trucking is possible with high strength materials which can reduce the vehicle weight within the existing envelope so as to increase payload capacity, and thereby reducing the number of trucks needed on the highways. Increased safety can be obtained by new brake materials and by incorporating highly shock absorbent materials in truck structures for improved control and crashworthiness. The DOE contacts are Joseph Carpenter (202) 586-1022, for automotive lightweighting materials and Sid Diamond (202) 586-8032, for high strength weight reduction materials.

The High Temperature Materials Laboratory (HTML) at the Oak Ridge National Laboratory is a modern research facility that houses in its six user centers, a unique collection of instruments for characterizing materials. It supports a wide variety of high-temperature ceramics and metals R & D. The HTML enables scientists and engineers to solve materials problems that limit the efficiency and reliability of advanced energy-conversion systems by providing access to sophisticated state-of-the-art equipment (which few individual companies and institutions can afford to purchase and maintain) and highly trained technical staff. The DOE contact is James Eberhardt, (202) 586-9837.

MATERIALS TECHNOLOGIES PROGRAM

AUTOMOTIVE PROPULSION MATERIALS

6. **TECHNICAL PROJECT MANAGEMENT**
   $150,000
   DOE Contact: R. Sullivan (202) 586-8042
   ORNL Contact: D. P. Stinton (865) 574-4556

The Automotive Propulsion Materials Program focuses on enabling materials technologies that are critical in removing barriers to the power electronics, fuel cell, and compression-ignition, direct-injection (CIDI) engine combustion and emissions control research prograMs. The objective of this effort is to assess the materials technology needs in each of these areas for hybrid electric or fuel cell vehicles, formulate technical plans to meet these needs and prioritize and implement a long-range research and development program.

Keywords: Advanced Heat Engines, Alloys, Automotive Applications, Carbon, Coordination, Metals, Management, Structural Ceramics

7. **LOW-COST, HIGH ENERGY PRODUCT PERMANENT MAGNETS**
$300,000
DOE Contact: R. Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: Y. S. Cha (630) 252-5899

The objective of this work is to develop a low-cost process for the fabrication of high strength NdFeB permanent magnets to enable significant size and weight reductions of traction motors for hybrid electric vehicles. A facility was established at Argonne National Laboratory for pressing permanent magnets in the high fields (9 T) of a superconducting solenoid. In FY 2003, we continued study on shape effect by focusing on smaller L/D ratios ($\leq$ 0.25), using the 1.125" die/punch set, where larger gain in energy product may be realized. However, all the samples cracked during ejection from the die. We investigated a number of factors which may have caused the cracking problem. The most likely culprit is trapped air in the sample. Another probable cause is that the design of the present die and press set cannot eject the sample under pressure, which could have prevented it from cracking. In attempts to alleviate the cracking problem, we completed conceptual designs of a vacuum die-filling and powder-pressing system and a compact ejection system under pressure. We continued the study on shape effect by using the electromagnetic computer code Opera and the results confirmed our previous conclusion that higher alignment field will help to reduce the field line distortion in the powdered compacts.

Keywords: NdFeB, Permanent Magnets, Superconducting Solenoids, Traction Motors

8. **CHARACTERIZATION OF PERMANENT MAGNETS**
$50,000
DOE Contact: R. Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: E. A. Payzant
(865) 574-4472

The purpose of this work is to quantify the relationship between processing parameters and the crystal chemistry and microstructure of NdFeB permanent magnets fabricated at Argonne National Laboratory and by commercial suppliers. The microscopic texture (alignment) of permanent magnets made in the Argonne axial-die press facility was characterized and correlated the alignment with macroscopic magnetic properties.

Keywords: NdFeB, Permanent Magnets

9. **CARBON FOAM FOR ELECTRONICS COOLING**
$300,000
DOE Contact: R. Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: Nidia Gallego
(865) 574-5220

The objective of this work is to collaborate with automotive partners to develop carbon foam heat exchanger and heat sink designs for high-power electronics that dissipate 30 W/cm^2 at temperatures of less than 60°C with lower cooling flow rates than current designs. Previous work has demonstrated that when graphite foam is utilized as the core material for a heat sink, the effective heat transfer can be increased by an order of magnitude compared to traditional materials and designs. A mathematical model was developed to predict the thermal performance of the foam in heat sink applications. However, the current model needs to be expanded to relate materials parameters (i.e., materials optimization) to the thermal properties for use in a power electronic thermal management system. Work will continue to evaluate and optimize carbon foam for conventional finned heat sinks applications. In addition, work addressing the fundamental understanding of the durability of the foam will be continued.

Keywords: Carbon Foam, Heat Sinks, Heat Transfer, Power Electronics, Thermal Management

10. **MECHANICAL RELIABILITY OF ELECTRONIC MATERIALS AND ELECTRONIC DEVICES**
$100,000
DOE Contact: R. A. Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: A. A. Wereszczak
(865) 576-1169

The objectives of this task are to assess and predict the mechanical reliability of electronic devices with emphasis on those used for automotive power electronics (e.g., capacitors) and to correlate the mechanical characterization of polymer film capacitors developed by Sandia National Laboratories (SNL) to the dielectric behavior.

More than 15 hydroxylated polystyrene (PVOH) films processed with different elastomer additives and annealing temperatures were mechanically characterized with a mechanical properties microprobe (elastic modulus, E, and hardness, H) and scratch testing and microstructurally characterized with scanning electron microscopy. The use of 4010 elastomer in PVOH resulted in lower E and H than the use of 5015 and TEGDE elastomers additives. Scratch testing results indicated that PVOH-4010 films tended to be more spall resistant and better suited for capacitor manufacturing than PVOH-5015 and PVOH-TEGDE filMs. These results were used by SNL in their down-selection of compositions to be fabricated in FY04.

Keywords: Power Electronics, Failure Analysis, Life Prediction, Mechanical Properties

11. **MICROWAVE-REGENERATED DIESEL ENGINE EXHAUST PARTICULATE FILTER TECHNOLOGY**
$200,000
DOE Contact: R. Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
Industrial Ceramic Solutions Contact: R. Nixdorf (865) 482-7552

The objective of this work is to develop a Diesel Particulate Filter that demonstrates greater than 95 percent capture efficiency and can be regenerated to within 95 percent of the new filter condition with the use of microwave energy. ICS developed a pleated ceramic fiber filter cartridge and demonstrated that it achieved 1/10th the exhaust backpressure of a conventional wall-flow particulate filters. The pleated filter completed efficiency testing on a 1.7-liter Mercedes engine in Oak Ridge National Laboratory's test cell to show greater than 96% removal of diesel PM down to 10 nanometers particle size. ICS designed, fabricated, and road-tested a pleated filter cartridge system and investigated microwave regeneration at engine idle condition on a 7.3-L Ford F-250 truck, with limited success of the microwave regeneration. Road testing of the pleated filter cartridge, without microwave-regeneration was conducted on the Ford F-250 diesel truck at a full range of engine operating conditions, showing good durability of the filter under high load conditions. The microwave filter system fuel penalty, as calculated from these test results, was an impressively low 0.3 percent.

Keywords: Carbon Particulates, Diesel, Filters, Microwave Regeneration

12. **MATERIAL SUPPORT FOR NONTHERMAL PLASMA DIESEL ENGINE EXHAUST EMISSION CONTROL**
$100,000
DOE Contact: Rogelio Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: S. D. Nunn (865) 576-1668

The objective of this work is to identify appropriate ceramic materials, develop processing methods, and fabricate complex-shaped ceramic components that will be used in Pacific Northwest National Laboratory (PNNL)-designed nonthermal plasma (NTP) reactors for the treatment of diesel exhaust gases. A supply of ceramic dielectric plates was fabricated for the assembly of stacks that will be used in an experimental NTP reactor that is to be tested on a small diesel engine. A prototype NTP reactor housing was fabricated from stainless steel sheet metal. Using the prototype, the final dimensions required to accommodate the dielectric stack and to attach it to the exhaust system of a 1.7L laboratory diesel engine can be determined. In laboratory tests, the bond strength of sealing glass compositions that are being evaluated for use in assembling the ceramic dielectric stacks was measured using a shear strength test apparatus. The two compositions, Ferro Corp. EG2964 and EG2998, had average shear strengths of 3034 psi and 2476 psi, respectively.

Keywords: Aftertreatment, Ceramics, Diesel, Gelcasting, Nonthermal Plasma

13. **FABRICATION OF SMALL INJECTOR ORIFICES**
$180,000
DOE Contact: R. A. Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: G. R. Fenske (630) 252-5190

Decreasing the size of fuel injector orifice holes enhances atomization of fuel in CIDI engines and thus presents a potential approach to achieve more stringent particulate emission standards. Currently, electrodischarge machining can routinely by used to fabricate orifices as small as 100mm in diameter. Ideally, however, the orifice diameter should be reduced to 50mm or less. The goal of this research is to develop an alternative approach to fabricating small fuel injector orifice nozzles by coating the inner surfaces of current mass-produced injector orifices–in other words, we will start with fuel injector nozzles/orifices that are currently produced in mass quantities, and develop coating processes to coat the inside surface to reduce the orifice to the size required. In the second year of the project, a reduction in orifice diameter from 0.2mm to 0.05mm was achieved on a bench scale. Current efforts are focused on establishing the feasibility of performing such coatings on a commercial scale, characterizing the changes in spray and combustion properties when using small-orifice nozzles in a diesel engine, and determining the vulnerability of the coating material to diesel fuel deposit formation.

Keywords: Fuel Injectors, Nozzles, Orifice, Coating

14. **TECHNOLOGY FOR PRODUCING SMALL HOLES IN ADVANCED MATERIALS**
$100,000
DOE Contact: Rogelio Sullivan (202) 586-8042
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: S. D. Nunn (865) 576-1668

The objective of this project is to explore new methods for forming ultra-small (<50mm) holes in advanced materials that may be used for fuel injector nozzles in diesel engines. Carbide-based cermets (ceramic/metallic composites) and high-temperature structural ceramics are candidate materials to be used in this study. Fine holes of various sizes were produced in a Ni_3Al-TiC cermet material by incorporating fine nickel wires in the cermet powder compact prior to sintering. Holes as fine as 26 μm in diameter were produced using this method. A plastic mold was designed to produce a controlled array of holes in gelcast ceramics having a fuel injector nozzle shape. Simulated nozzles of Al_2O_3 and ZrO_2 were cast with a circular array of eight holes in the tip of the nozzle shape. The holes were about 30 μm in diameter in the sintered ceramic parts. In a parallel study, coextrusion was examined and shown to be a viable forming method for producing a controlled array of fine holes in Al_2O_3 ceramic.

Keywords: Ceramics, Cermets, Diesel, Fuel Injectors, Gelcasting

15. **ELECTROCHEMICAL NO_x SENSOR FOR MONITORING DIESEL EMISSIONS**
    $370,000
    DOE Contact: R. A. Sullivan (202) 586-8042
    LLNL Contact: R. S. Glass (925) 423-7140
    LLNL Principal Investigator: L. P. Martin
    (925) 423-9831

The purpose of the proposed research is to develop technology for low cost, high sensitivity, on-board sensors for the detection of NO_x in diesel exhaust. The sensors will be based upon metal oxide/solid electrolyte technology which has demonstrated significant potential for the detection of hydrocarbon emissions in automobile exhaust. Sensor material and design will be optimized for an environment comparable to the exhaust stream of the CIDI engine. An oxide electrode material providing superior response has been identified for an amperometric-type NO sensor. The sensor operates at 650-750°, and has excellent NO sensitivity and a fast response time of 1 second or less. The high signal-to-noise ratio indicates a short-term sensitivity limit £25 ppm NO. Current efforts are focused on identification of sensing mechanism, and effects of electrode thickness and microstructure. The project is being performed in collaboration with Ford Research and Advanced Engineering and Oak Ridge National Laboratories. Critical path tasks for commercialization of the sensor are being shared by the three organizations (LLNL, ORNL and Ford) based on their expertise and support.

Keywords: NO_x, Electrochemical Sensor, CIDI, Diesel Exhaust

AUTOMOTIVE LIGHTWEIGHT VEHICLE MATERIALS

16. **LOW-COST HIGH PERFORMANCE WROUGHT ALUMINUM COMPONENTS FOR AUTOMOTIVE APPLICATIONS**
    $360,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069
    PNNL Contact: Mark Smith (509) 375-4478
    Laboratory Partners: LANL, PNNL
    Industry Partners: Alcoa

The objectives of this effort are: to develop electro-magnetic forming (EMF) technology that will enable the economic manufacture of automotive components from aluminum sheet; to experimentally validate stress-based forming limits; to validate enhanced formability through the application of non-proportional loading; and to demonstrate concept feasibility of infrared thermal forming of aluminum tubes.

Keywords: Aluminum, Sheet Forming, Extrusion, Hydroforming, Electromagnetic Forming, Thermal Forming

17. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVEAPPLICATIONS**
    $450,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069
    Laboratory Partners: LLNL, ORNL, SNL
    Industry Partners: USAMP (Ford, GM, Chrysler)

The objectives of this project are to develop the tools that will be used to enhance the application of cast magnesium components. These tools include: numerical simulation modeling to predict mold cavity fill and casting solidification for die cast components, simulation models that predict the cast component monotonic and cyclic properties, and development of non-destructive evaluation equipment, procedures, and process sensors.

Keywords: Magnesium, Cast Metals, Automotive, Die Casting, Simulation Modeling

18. **ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS**
    $475,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069
    PNNL Contact: Mark Smith (509) 375-4478
    Laboratory Partners: PNNL
    Industry Partners: USAMP (Ford, GM, Chrysler), Visteon

The objective of this effort is to develop a new low-cost process for the efficient on-site stir-casting of aluminum metal matrix composites suitable for the production of automotive components such as brake rotors and to demonstrate the effectiveness of the process on full scale components in vehicle tests. Other efforts focus on particulate reinforced powder metallurgy processes and applications.

Keywords: Metal Matrix Composites, Aluminum, Casting, Brake Rotors, Connecting Rods, Pumps

19. **TECHNOLOGY ASSESSMENT AND EVALUATION**
    $1,915,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
    PNNL Contact: Mark Smith (509) 375-4478
    ANL Contact: Ed Daniels (630) 252-5279
    Laboratory Partners: ANL, ORNL, PNNL

The objective of this effort is: to provide assessment of the cost effectiveness of various technologies; to evaluate the ability of the industrial infrastructure to accommodate emerging technologies; to verify, through modeling and analysis, that technologies developed will yield weight reductions commensurate with program goals; to provide guidance to program management as to appropriate investments for R&D funding; and to fund innovative research with small business.

Keywords: Cost, Infrastructure, Technical Management, Assessment

20. **ADVANCED JOINING TECHNOLOGIES**
    $1,350,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069; Dave Warren (865) 574-9693
    PNNL Contact: Mark Smith (509) 375-4478
    Laboratory Partners: LBNL, ORNL, PNNL
    Industrial Partners: Ford, General Motors, DaimlerChrysler

The objective of this effort is: to develop non-destructive evaluation and testing techniques that are sufficiently fast, robust in the manufacturing environment, accurate and cost-effective to be suitable or on-line inspection of spot-welded automotive structures; to develop joining technologies and evaluate joint performance for dissimilar aluminum and aluminum-steel materials in automotive applications; to develop coupled thermo-electric, mechanical-metallurgical models of electrode deformation during resistance spot welding of galvanized steel and aluminum; to develop new experimental methods and analysis techniques to enable hybrid joining as a viable attachment technology in automotive structures by evaluating composite/metal joints, time-dependent damage mechanisms, and environmental exposure for the ultimate development of practical modeling techniques that offer global predictions for joint durability; and to develop innovative attachment techniques for joining materials subjected to crash scenarios and to develop materials and joint test methods for joints and predictability tools.

Keywords: Joining, Dissimilar Materials, NDE, Aluminum, Galvanized Steel, Polymer Composites

21. **HIGH STRAIN RATE DEFORMATION OF MATERIALS**
    $1,050,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069
    Laboratory Partners: ORNL
    Industry Partners: AISI, Ford, General Motors, DaimlerChrysler

The objective of this effort is: to develop numerical methods and guidelines in order to realistically assess the influence that the properties of strain rate dependent materials exert in crashworthiness computations; to develop the capability of testing new lightweight materials at strain rates comparable to those observed in automobile crashes; to define the behavior of composite and metallic materials in the transition range from near static to highly dynamic failures; to develop experimental/analytical matrix for validation testing to evaluate constitutive models, work hardening effects, strain-rate sensitivity effects of selected high strength steels; and to develop materials and joint test methods for joints and predictability tools.

Keywords: Strain Rate, Crashworthiness, Numerical Modeling

22. **REINFORCED COMPOSITE MATERIALS, DURABILITY, AND ENABLING TECHNOLOGIES**
    $750,000
    DOE Contact: Joseph Carpenter (202) 586-1022
    ORNL Contact: Dave Warren (865) 574-9693
    Laboratory Partners: ORNL
    University Partners: University of Tennessee, University of Tulsa, University of Michigan, University of California-Santa Barbara, Wayne State University, Stanford University, University of Nottingham.
    Industry Partners: USAMP/Automotive Composites Consortium, Dow, Goodrich, Baydur Adhesives

The objective of this effort is to develop experimentally-based, durability driven guidelines to assure the long term environmental degradation, integrity of carbon-fiber-based polymeric composite automotive structures.

Keywords: Carbon-Fiber Reinforced Polymer Matrix Composites, Durability

23. **USAMP COOPERATIVE AGREEMENT**
$4,450,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORO Contact: Mary Rawlins (865) 576-0823
University Partners: University of Tulsa, University of Michigan, Alfred University, Georgia Tech University, University of Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham. Industry Partners: US Automotive Materials Partnership (DaimlerChrysler, Ford, GM), Goodrich, Baydyr Adhesives, Dow, Westmoreland, EKK, Entelechy, American Foundryman's Society, Mascotech, Stackpole Ltd., Valimet, Aluminum consultant's Group, Eck Industries, Meridian, Sparan Die Casting, Lunt Industries

The objectives of this project are to define and conduct vehicle related R&D in materials and materials processing. Projects include: Structural Cast Magnesium Development, Composite Intensive Body Structure Development, Crash Energy Management, High Volume Processing of Composites, Hydroforming of Aluminum Tubes, Adaptive Flexible Binder Control for Robust Stamping of Aluminum Sheet, Long Life Electrodes for Resistance Spot Welding of Aluminum Sheet Alloys and Coated High Strength Steels, Magnesium Powertrain Die Cast Components, Plasma Arc Welding of Lightweight Materials, Warm Forming of Aluminum, High Strength Steel Stamping (Springback Predictability) Hydroforming and Lubricants for High Strength Steels, Strain Rate Characterization of High Strength Steels, High Strength Steel Tailor Welded Blanks. Projects are conducted by multi-organizational teams involving USAMP members, automotive suppliers, universities, and private research institutions.

Keywords: Polymer Composites, Aluminum, Magnesium, Fiber Preforming, Adhesive Bonding, Rapid Prototyping, High Strength Steel, Forming, High Volume Processing, Stamping, Die Casting, Welding, Spot Welding

24. **DEVELOPMENT OF LOW-COST CARBON FIBER**
$1,807,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: ORNL
University Partners: Clemson University, Virginia Technological University
Industry Partners: USAMP/Automotive Composites Consortium, AKZO Fortafil Fibers, Amoco, Westvaco, Hexcel Corporation

The objective of this effort is to conduct materials research to lead to the development of low cost carbon fiber for automotive applications. Research includes investigation of alternate energy deposition methods and alternate precursors for producing carbon fiber as well as the development of improved thermal processing methods and equipment for fiber manufacture. This work examines the fiber architecture and manufacturing issues associated with carbon fiber usage to take advantage of the high strength and modulus of carbon fiber while minimizing the effects of its low strain-to-failure. The ultimate goal of this effort is to reduce the cost of commodity grade carbon fiber to $3-5 per pound.

Keywords: Polymer Composites, Durability, Processing, Low Cost Carbon Fiber, Microwave Processing, Precursors

25. **RECYCLING**
$1,100,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
ANL Contact: Ed Daniels (630) 252-5279
Laboratory Partners: ANL
Industry Partners: Vehicle Recycling Partnership (Ford, GM, DaimlerChrysler)

The objectives of this effort are: to investigate cost-effective technologies for recycling polymer composites; and to establish priorities for advanced recycling initiatives and provide technical oversight to ensure that priority goals and objectives are accomplished.

Keywords: Recycle, Polymer Composites

26. **STRUCTURAL RELIABILITY OF LIGHTWEIGHT GLAZING ALTERNATIVES**
$315,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: M. A. Khaleel (509) 375-2438
Laboratory Partners: PNNL
Industry Partners: Visteon

The objective of this effort is to develop advanced numerical modeling and simulation tools to evaluate the structural reliability of lightweight thin glazing designs for automotive applications.

Keywords: Glazing, Structural Reliability

27. **HIGH RATE PROCESSING TECHNOLOGIES FOR POLYMER COMPOSITE MATERIALS**
$1,493,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
Laboratory Partners: ORNL
Industry Partners: USCAR (DaimlerChrysler, Ford, General Motors).

The purpose of this effort is to develop technologies to cost effectively process composite materials into automotive components, integrate these technologies into demonstration projects that display cost effective use of composites that can be manufactured in automotive factories, develop advanced vehicle system designs based on composite materials to both define future research needs and demonstrate the technical and economic viability of developing technologies. A portion of this effort is devoted to developing the next generation programmable processing machine.

Keywords: Automotive, Polymer Composites, High Rate Processing, Focal Project Design

HEAVY VEHICLE PROPULSION MATERIALS

28. **SMART MATERIALS FOR FUEL SYSTEM ACTUATORS**
$400,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
DDC Contact: Craig Savonen (313) 592-5315

The objective of this effort is to develop advanced diesel engine fuel injection systems based on smart materials, such as piezoelectrics. Advanced fuel systems may control the fuel injection event such that several controlled injections are made for each combustion cycle, thus facilitating the control of combustion to optimize the efficiency and emissions from the engine. The effort includes fuel injector design and bench and engine testing. The incremental performance advantages of applying advanced material actuation to either of the candidate actuator systems will be quantitatively evaluated by a combination of baseline experimental results, material characterization, and advanced electro-mechanical-hydraulic analysis.

Keywords: Fuel Systems, Piezoelectric Actuators

29. **COST-EFFECTIVE SMART MATERIALS FOR DIESEL ENGINE APPLICATIONS**
$300,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

Work performed in FY 2003 has involved modifying commercial PZT powders with chemical additives and attrition milling to allow sintering of the PZT materials between 900 and 950˚C. These sintering temperatures should allow the use of silver interlayer electrodes in the multilayer actuators. The primary work in FY 2004 will focus on making multilayer PZT stacks using inner electrodes fabricated from silver or silver doped with other materials to adjust for thermal mismatch during sintering. Other areas of keen interest are to strengthen and/or toughen PZT materials with nano-metal or ceramic additives. Finally a test fixture will be fabricated to compress and measure the stroke of PZT multiplayer parts that will be fabricated.

Keywords: Fuel Systems, Piezoelectric Actuators

30. **MANUFACTURING TECHNOLOGY FOR CERMET COMPONENTS**
$75,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
SIUC Contact: Dale Wittmer (618) 453-7006

The purpose of this work is to investigate the potential of low-cost manufacturing processes for ceramic and cermet diesel engine components. The primary task is to develop cost-effective processing, forming, and sintering methodologies for cermet and ceramic formulations used by industrial engine manufacturers. During this funding cycle, we will continue to use our low-pressure injection molder to form several batches of intermetallic bonded TiC. The formed cermets will then be sintered by both continuous sintering at SIUC and by the V-LPHIP process at ORNL. We intend to continue this work to the point of being able to produce near net shape parts for use in diesel engines.

Keywords: Cermets, Intermetallics, Manufacturing Technology

31. **INTERMETALLIC-BONDED CERMETS**
$100,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The goal of this task is to develop high strength, high toughness materials that can be sintered to near-net-shape for diesel engine applications, specifically for fuel delivery systems and wear components (e.g., valve seats and turbocharger components). This will require materials which have a minimum hardness of 11 GPa and a thermal expansion coefficient of up to 12×10^{-6}/˚C for temperatures up to ~600˚C to minimize thermal mismatch with metallic alloys. The material should also have excellent corrosion resistance in a diesel engine environment, flexure strength in excess of 700 MPa, and fracture toughness >10 MPa√m to ensure long term reliability. The material should also be compatible with metallic alloys and exhibit negligible wear in combination with them. Finally, the total material processing costs for these advanced materials should be competitive with competing technologies such as TiN or other ceramic coatings on high-speed tool steels.

Keywords: Cermets, Intermetallics, Fuel Systems

32. **HIGH-TOUGHNESS MATERIALS**
$300,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of the effort is to develop high toughness materials that are also low cost. TiC-Ni_3Al composites have shown a combination of superior physical properties and mechanical behavior using conventional powder processing methods. Previously, the general property envelope has been studied and the compositions refined. Further processing studies are needed to examine lot-to-lot variation using statistically designed experiments, determine compaction behavior, assess dimensional control during sintering, identify suitable binders which will not add carbon ash during sintering, and develop a viable and cost-effective source of NiAl powder. The project activities will be in close association with CoorsTek Inc. (a parts supplier) for scale-up of the processing, and Cummins Engine Co. for rig testing of fabricated parts.

Keywords: Cermets, NiAl, TiC

33. **MATERIALS FOR EXHAUST AFTERTREATMENT**
$400,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Caterpillar Contact: Lou Balmer (309) 578-4468

This program covers the following technologies:
1) Lean-NO_x Catalysis - Because of the inherently low hydrocarbon concentration in diesel exhaust, any NO_x reduction catalyst will require the addition of supplemental reductant to achieve performance goals. From a diesel engine user's standpoint, the best reductant to use in conjunction with aftertreatment systems is diesel fuel. Therefore, emphasis will be placed on research and development on catalyst aftertreatment technologies that can utilize diesel fuel as a reductant to reduce NO_x including Lean-NO_x and Plasma Assisted Catalysis technologies. 2) NO_x Sensor - In most aftertreatment strategies, multiple NO_x sensors will be required to monitor exhaust NO_x levels as an on-board diagnostic tool and to control the aftertreatment device/engine for maximum fuel efficiency. The research will continue to focus on improving durability and response time of current state of the art sensors, in particular, amperometric type sensors. Further research will focus on alternative technologies for sensing NO_x in the diesel exhaust environment.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

34. **CATALYST CHARACTERIZATION**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Cummins Contact: Roger England (812) 350-5246

In order to meet the 2007 emission requirements for diesels, it will be necessary to have a catalyst system in diesel engines. Currently, no commercial technologies are available to meet these standards. Consequently, Cummins Inc. is developing their own system and seeks the assistance of Metals and Ceramics Division at the Oak Ridge National Laboratory (ORNL) with its materials characterization effort. The purpose of this effort is to produce a quantitative understanding of the process/ product interdependence leading to catalyst systems with improved final product quality, resulting in diesel emission levels that meet the 2007 emission requirements. In the FY03 effort, baseline characterizations were done to provide reference points. The location and dispersion of active catalytic elements in the washcoat were verified, and the temperature dependence and thermal stability of the adsorbed species was determined.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

35. **DEVELOPMENT OF NO_x SENSORS FOR HEAVY VEHICLE APPLICATIONS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The NO_x sensor is an enabling technology which will promote the advancement of both lean burn gasoline engines and diesel engines by permitting improved engine control, along with the mandated on-board diagnostics. This task seeks to develop catalytically selective electrodes that will facilitate the development of simple resistive-type (mixed potential) NO_x and ammonia sensors. The research will follow the logical progression from: the catalytic evaluation of mixed conducting oxide powders; the evaluation of the kinetics at the surfaces of these materials under the influence of applied electric potential; and finally, the development of low-cost, resistive sensors based on materials developed.

Keywords: Sensors, No_x, Exhaust Aftertreatment

36. **ELECTRON MICROSCOPY FOR CHARACTERIZATION OF CATALYST MICROSTRUCTURES AND DEACTIVATION MECHANISMS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of the research is to use analytical and high-resolution transmission electron microscopy (TEM) to characterize the microstructures of emission-control catalysts. Catalyst research places emphasis on relating microstructural changes to performance of diesel NOx-reduction catalysts. This research is focused on understanding these changes through TEM studies of experimental catalyst materials reacted in an ex-situ catalyst reactor system especially constructed to allow appropriate control of the reaction conditions and the transfer of the sample between reactor and microscope. A secondary objective is to gain a better understanding of the structures of catalytic materials starting from the atomic level, by studying model catalyst systems comprising heavy metal species on oxide supports.

Keywords: TEM, Catalyst, Microstructure

37. **MICROSTRUCTURAL CHANGES IN NO_X TRAP MATERIALS UNDER LEAN AND RICH CONDITIONS AT HIGH TEMPERATURES**
$100,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of this research is to study the microstructural changes that accompany the reaction of NO_x, under lean and rich conditions at high temperatures, with trap materials synthesized in our laboratories at ORNL. The samples for this study will be both 1) the model NO_x traps $Pt/BaO.6Al_2O_3$ where $BaO.6Al_2O_3$ is prepared by impregnation, co-precipitation, or sol-gel processing, and 2) the fully formulated NO_x traps $Pt/BaO.6Al_2O_3$-La_2O_3-CeO_2-ZrO_2. It is important to point out that most of the thermal stabilization effort has been limited to finding thermally stable NO_x absorber components because the accepted mechanism for the thermal aging of NO_x traps assumes that NO_x absorbers form aluminates on aging. Recent results suggest that it is possible to reverse aging if it is due to the formation of aluminates. Furthermore, NO_x traps will also be examined where precious metals have been partially replaced by base metals to improve the trap's thermal stability. The work will be carried out in collaboration with colleagues at Ford Research Laboratory, where the samples for Tasks I-III are being evaluated for NO_x trap efficiency. The fresh samples prepared in Task IV will also be evaluated using bench reactors and analysers at FRL, until an equivalent capability is established at ORNL.

Keywords: NO_x Trap Materials, NO_x Absorber Components

38. **AFTERTREATMENT CATALYSTS MATERIALS RESEARCH**
$85,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Cummins Contact: Randy Stafford (812) 377-3279

This effort addresses research in two major areas of diesel exhaust aftertreatment: abatement of diesel soot and reduction of No_x. Abatement of diesel soot research focused on the following issues: developing novel catalytic materials for efficient soot oxidation, the effect of microwave heating on the efficiency of soot generation, and developing advanced techniques for probing the degradation of soot filters. The following tasks were performed:

- Combinational synthesis of catalysts
- Synergistic potential of mixed oxides
- Filter cavity geometry for optimized heating
- Microreactor catalyst testing
- Microreactor probing of catalyst deterioration

The major technology barrier that was addressed in the reduction of No_x area is sulfur poisoning of NO_x absorbers. The sulfation and desulfation of NO_x absorber materials will be investigated using a suite of flow-reactor tools and surface analysis tools to understand the underlying materials changes that affect performance.

Keywords: Diesel Engine, Exhaust Emissions, Particulate Emissions

39. **ADVANCED MATERIALS FOR LIGHTWEIGHT VALVE TRAIN COMPONENTS**
$189,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Caterpillar Contact: Mark Andrews (309) 578-3896

The Advanced Materials for Lightweight Valve Train Components Program plans to design and fabricate prototype engine valves from high temperature advanced materials. The design of these valves will be based on established probabilistic design methodologies (e.g., NASA/CARES Life and Honeywell's CERAMIC and ERICA computer codes). The testing of the prototype valves will be accomplished on an in-house designed valve test rig.

Keywords: Valves, Diesel Engines, Life Prediction

40. **ENGINEERED SURFACES FOR DIESEL ENGINE COMPONENTS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Caterpillar Contact: Brad Beardsley (309) 578-8514

Engine testing of thermal sprayed coatings has demonstrated that their use as thermal barriers and wear coatings can reduce fuel consumption, reduce wear and reduce component temperatures. The durability of thermal sprayed coatings, particularly thermal barrier coatings, remains as the major technical challenge to their implementation in new engine designs. New approaches to coating design and fabrication will be developed to aid in overcoming this technical hurdle. New laser technology of surface dimpling, cleaning and laser assisted spraying will be applied to enhance adherence and increase coating strength. Refinements of current seal coating technologies will be developed to further enhance the durability of the coating structure. New quasi-crystalline materials will be evaluated as thermal barrier coatings as well as wear coatings for ring and liner applications and as low friction coatings for camshafts and crankshafts. Plasma spraying, D-Gun and HVOF processing with new engineered powders will be used to develop these new coatings.

Keywords: Thermal Barrier Coatings, TTBC, Plasma Spraying

41. **CERMET MATERIALS FOR DIESEL ENGINE WEAR APPLICATIONS**
$125,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Cummins Contact: Randy Stafford (812) 377-3279

Earlier work at Cummins on cermet composites for wear applications produced encouraging data for several compositions of titanium carbide-nickel aluminide and tungsten carbide-cast iron materials. This data showed that the TiC/Ni_3Al had sliding wear properties near magnesia stabilized zirconia and the WC/cast iron had sliding wear properties better than conventional hardened steel and cast iron. The advantages shown by the cermet are the ability to produce a near net shape component, machinability by electrodischarge machining (EDM) and reduced wear of the counterface. An additional advantage of the WC/cast iron is potential for low cost components. The program proposed is a follow-on to the previous work and will focus on optimization of the compositions and microstructures and evaluation of the materials from multiple production batches. The work on TiC/Ni_3Al will concentrate on one composition with up to 10 batches of powder manufactured (approximately 1 kg batch size), followed by characterization of the powder and pressing and sintering of test bars. The density, strength, and wear properties will be compared for each batch. The work on WC/cast iron will include: optimizing the volume fraction of WC and developing a robust preform for casting and optimizing the cast iron matrix hardness and toughness (trials with grey iron and ductile iron material).

Keywords: Tribology, Wear, Cermet

42. **MECHANICAL CHARACTERIZATION**
$80,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
NCA&T Contact: Jag Sankar (336) 256-1151

This project consists of the following four parallel tasks:

Task 1 - Thermal Barrier Protective Surface Coating. A basic scientific understanding of thermal barrier protective surface coating (TBC) to promote high-temperature performance and the effects of surface flaws and oxidation at elevated temperatures for these materials shall be initiated and carried out.

Task 2 - Nano-Engineered Smart Materials. Pulsed Laser Deposition (PLD) technique gives a unique approach in developing novel oxides. NCA&T is developing a novel smart thin film processing method based upon pulsed laser deposition to process nanocrystalline materials with accurate size and interface control with improved mechanical and magnetic properties. Processing parameters, structure /property correlation and change in magnetic characteristics shall be investigated.

Task 3 - Solid Oxide Thin FilMs. Zirconium oxide has been extensively used in tribological and thermal barrier coatings for many years. NCA&T shall continue to develop a liquid fuel combustion CVD technique for solid oxide thin film deposition. The processing parameters shall be optimized for the system. We shall also conduct research related to controlling grain size (nano to micron grain size) to observe the effects on fuel cell materials property.

Task 4 - Property Characterization. Mechanical property characterization through appropriate methods including nanohardness technique and full range of microscopy (macro to atomic level) and fractography work shall be a part of all tasks discussed above.

Keywords: Thermal Barrier Coatings, Nano Materials, Thin Films, Fuel Cells

43. **NDE OF DIESEL ENGINE COMPONENTS**
$210,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
ANL Contact: Bill Ellingson (630) 252-5068

The purpose of this work is to characterize machining damage in structural ceramic valves for diesel engines using various nondestructive evaluation (NDE) methods. One primary NDE method to be addressed is elastic optical scattering. The end target is to demonstrate that data produced by this method can be correlated to damage as well as used for predicting material microstructural and mechanical properties. There are three tasks to be carried out: 1) characterize surface/subsurface defects and machining damage and correlate NDE data with mechanical properties for flexure-bar specimens of several silicon nitrides used for valves; 2) assess/evaluate ceramic valves to be run in a single cylinder test engine; and 3) evaluate surface-damage healing by laser glazing on machined surfaces. This proposed work is a cooperative program with Caterpillar Inc.

Keywords: NDE, Nondestructive Evaluation, Ceramic Valves

44. **DURABILITY OF DIESEL ENGINE COMPONENT MATERIALS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of this effort is to enable the selection and development of durable, lower-friction moving parts in diesel engines for heavy vehicle propulsion systems through the systematic evaluation of promising new materials, surface treatments, composites, and coating technologies under component-specific conditions. Specifically, the approach involves test method development, microstructural analysis, behavioral mapping, and modeling. In FY 2002, a test method was developed to study the friction and wear characteristics of candidate exhaust gas recirculation (EGR) system materials. A series of carefully selected commercial alloys, ceramics, and experimental materials were evaluated for their high-temperature scuffing behavior. In FY 2003, this effort was extended to include an investigation of the scuffing of fuel injector component materials. Innovative testing techniques were developed to produce and measure the fine-scale surface damage that is observed in diesel engine fuel system parts.

Keywords: Tribology, Friction and Wear, Scuffing

45. **LIFE PREDICTION OF DIESEL ENGINE COMPONENTS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

There has been considerable interest in the extensive potential use of advanced ceramics and intermetallic alloys for applications in advanced diesel engine systems because of their superior thermomechanical properties at elevated temperatures. This interest has then focused primarily on research aimed at characterization and design methodology development (life prediction) for advanced silicon nitride ceramics and TiAl alloys in order to manufacture consistent and reliable complex-shaped components for diesel engine applications. The valid prediction of mechanical reliability and service life is a prerequisite for the successful implementation of these advanced materials as internal combustion engine components. There are three primary goals of this research project, which contribute toward successful implementation: the generation of mechanical engineering database from ambient to high temperatures of candidate advanced materials before and after exposure to simulated engine environments; the microstructural characterization of failure phenomena in these advanced materials and components fabricated from them; and the application and verification of probabilistic life prediction methods using diesel engine components as test cases. For all three stages, results will be provided to both the material suppliers and component end-users to refine and optimize the processing parameters to achieve consistent mechanical reliability, and validate the probabilistic design and life prediction of engine components made from these advanced materials.

Keywords: Life Prediction, Mechanical Characterization

46. **LOW-COST MANUFACTURING OF PRECISION DIESEL ENGINE COMPONENTS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

Cost-effective machining processes are needed to ensure the widespread use of high-performance materials in engine components. Such components are typically made from ceramics, ceramic-composites, and intermetallic materials. ORNL has developed instrumented systems for studying the fundamentals of machining processes needed to make precision components from these materials. In the past, emphasis has been placed on grinding, since this is usually the process of last resort for shaping difficult-to-machine materials. However, because there is also a need to apply other machining processes such as such as turning, milling, and drilling to these advanced materials, we are expanding our capabilities to include these processes. In addition, non-destructive inspection techniques are being developed to verify that mechanical properties are not being degraded by the machining processes. These efforts are best accomplished by working directly with engine manufacturers, suppliers, machine tool builders, and the academic community.

Keywords: Machining, Inspection, Grinding, Turning, Milling, Drilling

47. **ADVANCED MACHINING AND SENSOR CONCEPT**
$75,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Univ. of Michigan Contact: Albert Shih (919) 515-5260

Cost-effective machining of cermets is critical to promote the application of this wear-resistant, difficult-to-machine material. The grinding temperature and temperature distribution inside a diesel exhaust filter during regeneration are important to understand the conditions and performance of the process. Titanium, another difficult-to-machine material, has the potential to be widely used as a lightweight material for transportation applications, if machining costs to achieve the final shape can be reduced. This research will explore the cylindrical wire electrical discharge machining (EDM) of cermets, investigate the infrared-based, non-contact temperature measurement for grinding and diesel exhaust filter, and study the machining of titanium-based alloys.

Keywords: EDM, Temperature Measurement, Titanium

48. **ADVANCED CAST AUSTENITIC STAINLESS STEELS FOR HIGH-TEMPERATURE EXHAUST COMPONENTS**
$160,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of this work is to evaluate cast austenitic stainless steels as alternate materials for SiMo ductile cast iron currently used in many diesel engines for exhaust manifold and turbocharger housing components. Cast stainless steels must withstand prolonged exposure at temperatures of 750˚C or above, as well as survive the severe thermal cycling from such high-temperatures to near room-temperature. This project has tested commercially available cast alloys and has developed several new modified cast stainless steels with significantly enhanced performance relative to SiMo cast iron. The ultimate objective is a high-performance, reliable, and cost-effective exhaust component material.

Keywords: Austenitic Stainless Steel, Ductile Cast Iron, Exhaust System

49. **TiAl NANOLAMINATE COMPOSITES**
$75,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
LLNL Contact: Luke Hsiung (925) 424-3125

This research seeks to fabricate and design TiAl alloys with desired microstructures and adequate alloying composition for advanced Diesel engine applications. The primary goals are 1) to exploit thermomechanical (hot extrusion) processing technique to fabricate two-phase TiAl alloys with refined lamellar microstructures, 2) to experimentally verify microstructural stability and creep resistance of the alloys, and 3) to investigate fundamental interrelationships among microstructures, alloying additions, and creep properties of the alloys so as to achieve the desired performance of the alloys for high-temperature applications.

Keywords: Titanium, Titanium Aluminide, Lamellar Microstructure

50. **SYNTHESIS OF POWDERS FOR TITANIUM CARBIDE/NICKEL ALUMINIDE CERMETS**
$48,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
University of Colorado Contact: Alan Weimer (303) 492-3759

The objectives of this project are: 1) to synthesize submicron TiC particles by rapid carbothermal reduction, and 2) to develop a better understanding of monolithic nickel aluminide synthesis and the potential for in-situ composite TiC/Ni_3Al synthesis. Preliminary work using a high-temperature, thermogravimetric analyzer has indicated that fine TiC powders of high purity can be synthesized with fast kinetics, indicating that "rapid carbothermal reduction" (RCR) using a transport tube reactor may be feasible. Since RCR processing is a commercial process for producing tungsten carbide (WC) and since the synthesis of TiC and WC are similar, the RCR synthesis route may provide the best opportunity for commercial high quality TiC. Very little work has been done to understand the kinetics and effect of reactants on the synthesis of nickel aluminide (NiAl and Ni_3Al) powders. In addition, it would be desirable to utilize the exothermic heat of reaction from the nickel aluminide reaction to drive the endothermic carbothermal reduction synthesis of titanium carbide. The reactions will need to be compatible in terms of reaction rate and temperature. The temperature of reaction, the purity and size of the starting reactants, and the reactant composition will impact the reaction rate and quality of the products.

Keywords: Powder Synthesis, Titanium Carbide, Nickel Aluminide, Carbothermal Reduction

51. **DIESEL EXHAUST GAS RECIRCULATION CORROSION EFFECTS**
$50,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

In order to reduce NOx emissions, exhaust gas recirculation (EGR) systems have been deployed in diesel engines. This approach reduces the peak combustion temperatures and hence, NOx emissions. The use of EGR can lead to accelerated corrosion that is considered to be associated with the formation of sulfuric acid. While it has been observed that corrosion tends to follow the dewpoints, there are indications of maxima in corrosion rates with dewpoint temperature. Two regimes have been identified. The first regime is in the temperature range between the dewpoints of the acid that forms and that of water where strong acid is formed, and the second regime is below the water dewpoint where very weak acid is formed. Both of these acid concentrations, strong (50 - 70 percent) or very weak (500 ppm), are very aggressive corrodents of the proposed materials of containment, aluminum and steel alloys. The objective of this task is to assess the effect of the various operating regimes controlled by engine parameters such as fuel rate, fuel composition, EGR fraction, and engine coolant temperature, on the corrosion rates of materials of construction. The data and information generated will enhance materials selection.

Keywords: Corrosion, EGR

52. **LASER SURFACE TEXTURING OF LUBRICATED CERAMIC PARTS**
$50,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of this effort is to evaluate the frictional benefits of placing laser dimple patterns on boundary-lubricated ceramic surfaces. This project is part of a joint Argonne National Laboratory/ORNL effort to ascertain the benefits of laser surface texturing (LST), a process developed by Surface Technologies, Ltd., Israel. That process uses a computer-controlled laser to produce a pattern of shallow rounded dimples on bearing surfaces. Based on calculations, preliminary tests, and limited field trials, the developer claims that LST enhances the ability of a lubricated surface to establish a load-bearing hydrodynamic film that decreases friction relative to a non-dimpled surface. The ORNL portion of this joint effort is focused on two aspects of LST: 1) conducting reciprocating tests of ceramic surfaces using lubricating fluids with various viscosities, and 2) determining the microstructural changes that are associated with the LST process. In FY 2002, LST surfaces of zirconia and silicon carbide were obtained and friction-tested against silicon nitride under reciprocating sliding contact in water, mineral oil, and diesel oil. The viscosity and frequency of oscillation was shown to influence the degree by which dimpling reduced friction. Electron microscopy, both scanning and transmission, revealed microstructural effects of the laser treatment process on the bearing surfaces of both ceramics.

Research in FY 2003 will complete characterization of both the tribological and microstructural implications of applying LST to ceramic bearing surfaces.

Keywords: LST, Laser Surface Texturing

53. **LOW COST TITANIUM FEEDSTOCK CONSOLIDATION PROCESS**
$100,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Dynamet Technology Contact: Stanley Abkowitz (781) 272-5967

Dynamet Technology will produce nine prototype Ti-6Al-4V billets from low cost raw materials (i.e., titanium powder and master alloy powder blended with specially processed fine Ti-6Al-4V alloy turnings). These alloy blends will be consolidated to high density billet feedstock by cold isostatic pressing, vacuum sintering and in specific cases include hot isostatic pressing. The billet feedstock will be evaluated for densification and microstructure.

Keywords: Titanium, Powder Metallurgy

54. **HIGH DENSITY INFRARED SURFACE TREATMENT OF MATERIALS FOR HEAVY-DUTY VEHICLES**
$70,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

High Density Infrared (HDI) technology is relatively new to the materials processing area and is gradually being exploited in materials processing. The HDI processing facility at ORNL utilizes a unique technology to produce extremely high-power densities of 3.5 kW/cm^2 with a single lamp, which is currently the most powerful one in the world. Instead of using an electrically heated resistive element to produce radiant energy, a controlled and contained plasma is utilized. The advantages of the technology include: compared to laser technology, it can cover large areas; consists of short wavelength radiation (0.2-1.2 μm); fast heating and cooling rates; capable of attaining very high temperatures; potential for continuous processing.

Since the technology is relatively new, its utility for the surface treatment of materials for applications in heavy-duty vehicles will be explored. In most cases, the need for wear resistance, or corrosion resistance, or high strength is only necessary in selected areas of the part that is exposed to the working environment or under high stress. Therefore, it would be desirable to use materials that are lighter or less expensive for the bulk of the part and only have the appropriate surface properties where required. The project using HDI technology will be exploratory and will examine a couple of approaches on surface modification that would be of interest to materials for heavy-duty vehicles. The first area would be in the application and formation of adherent, wear/corrosion resistant coatings. The initial tests would be based on hardmetal compositions applied on to iron-based parts that are currently used. The other area that would be examined in the initial study would be the treatment of plasma-sprayed coatings that had been put on iron-based substrates. These types of coatings are presently used extensively in heavy-duty vehicles. Previous work had shown that HDI surface treatment of certain ceramics resulted in columnar grain growth at the surface. Thus, the HDI has the potential to modify the plasma sprayed microstructure to one that is columnar in nature. Such coating microstructures are believed to have better properties than the plasma sprayed coatings. In addition, the HDI approach would be more cost-effective than other competitive processes such as physical vapor deposition. Based on these exploratory studies, further research on the utilization of HDI technology could be ascertained.

Keywords: Infrared Processing, Surface Treatment

55. **HIGH TEMPERATURE ALUMINUM ALLOYS**
$90,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Cummins Contact: Randy Stafford (812) 377-3279

Task 1 - A ternary phase aluminum alloy utilizing rare earth metals to provide precipitate size control and stability. Limited information on these alloys from UTRC indicates high temperature strength and stability; however, the predicted cost of the alloy is high. Ongoing work is needed to determine if there are additional rare earth (or other metal) elements which produce the beneficial properties at a reasonable cost. Task 1 work will concentrate on development of ternary phase compositions with modeling of the phase diagram and evaluation of properties for alloys identified as potential candidates.

Task 2 - A conventional aluminum alloy which has a modified chemistry by a process developed at NASA-Huntsville. The elevated temperature properties reported by NASA are attractive, but it is preferable for Cummins to use alloys with lower silicon content. Eck Industries has purchased the license for the NASA developed technology on these high silicon casting alloys and has expanded the range to include conventional low silicon casting alloys. Limited testing of these modified conventional low silicon alloys at Cummins has not shown the property improvement anticipated. Task 2 work will concentrate on property measurements to characterize the material. Different alloy compositions and heat treatments will be investigated for the optimum strength, toughness and fatigue strength.

Task 3 - A particulate loaded aluminum alloy. The nano-phase particulate at 50 volume percent provided high temperature strength, however, the alloy can only be forged or squeeze cast so complex shape capability is limited. Task 3 will concentrate on property measurements to characterize the material. Casting modifications will also be investigated to determine shape capability for the alloy.

Keywords: Aluminum, Creep, Low-Cycle Fatigue

56. **ROLLING CONTACT FATIGUE**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
NIST Contact: Said Jahanmir

During the coming year we will develop test methods for evaluating the contact damage behavior of ceramics under rolling and sliding conditions that simulate those of cam roller followers, valves and valve seats. The recommendations of the Contact Damage Working Group members will guide our studies. We will involve international members through our participation in a new IEA Annex III. From the many recommendations of our working group, we will focus on two main areas: fundamental understanding of the nature of contact damage in RCF and potential standardization of the 3-ball-on-rod RCF test. If sufficient technical interest and capability exist, we will initiate a formal standard development.

Keywords: Contact Damage, IEA, Rolling Contact Fatigue

57. **IEA IMPLEMENTING AGREEMENT FOR A PROGRAMME OF RESEARCH AND DEVELOPMENT ON ADVANCED MATERIALS FOR TRANSPORTATION APPLICATIONS**
$200,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832

The objective of this project is the cooperative assessment of new technologies for materials fabrication, surface modification, and advanced materials characterization techniques of interest to the transportation sector. The mechanisms for this cooperative effort include information exchanges and joint research tasks. Specific topics currently under consideration are characterization of thin coatings for wear and thermal protection, contact damage assessment, development of materials for hydrogen storage, and assessment of novel surface modification techniques for improved wear behavior. The active members in this IA are United States, Japan, and Germany.

Keywords: IEA, Materials Characterization

58. **TESTING STANDARDS**
$105,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
NIST Contact: George Quinn (303) 492-3759

Work focused on the following American Society of Testing and Materials (ASTM) and International Organization for Standards (ISO) standards: flexural strength standard C 1161, fracture toughness standard C 1421, fractographic analysis standard C 1322, Surface Crack in Flexure (SCF) ISO test method standard and new flexural strength standards for cylindrical rods.

Keywords: Standards, ASTM, Fracture Toughness, Flexural Strength

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

59. **DESIGN, ANALYSIS AND DEVELOPMENT OF LIGHTWEIGHT FRAMES FOR TRUCK AND BUS APPLICATIONS**
$891,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Autokinetics, DaimlerChrysler, Alcoa, Tower Automotive

The objective of this project is to develop concepts for lightweight frames for Class 1 and 2 trucks and buses, develop and implement low-cost manufacturing technologies, and validate concepts on full size vehicles. Materials under consideration include aluminum, high strength steels, and stainless steels.

Keywords: Frames, Manufacturing, Lightweight, Trucks, Buses

60. **DEVELOPMENT OF ADVANCED CASTING TECHNOLOGIESMETAL COMPRESSION FORMING (MCF) FOR PRODUCTION OF HIGH INTEGRITY TRUCK COMPONENTS**
$715,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 375-4478
Laboratory Partners: ORNL, PNNL, Albany Research Labs
Industry Partners: Freightliner, PACCAR, Alcoa, Eck Industries

The objectives of this project are: to develop and integrate the necessary hardware and production procedures to implement advanced casting technologies to a level capable of producing high-integrity parts at rates and volumes necessary for truck and automotive applications.; to develop the necessary understanding and technology to cast large structural components for Class 8 truck cabs; and to develop modeling and design capabilities for optimizing steel castings for heavy vehicle applications to reduce weight without sacrificing performance.

Keywords: Aluminum Alloy, Casting, Truck, Automotive, Steel Castings

61. **ADVANCED FORMING TECHNOLOGIES FOR LIGHTWEIGHT ALLOYS**
$550,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: LANL, PNNL, INEEL, ORNL

The objective of this project is to evaluate new forming technologies for processing lightweight alloys, to use the new process to achieve improved microstructure, properties, performance, and control in the production of components for heavy vehicles.

Keywords: Extrusion, Lightweight Alloys, Forming, Superplastic Forming, Thermal Forming, Magnesium, Aluminum

62. **DEVELOPMENT OF CARBON MONLITHS FOR SAFE, LOW PRESSURE ADSORPTION STORAGE AND RELEASE NATURAL GAS**
$550,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of this project is to develop and test monolithic carbon adsorbant materials for the storage of natural gas in heavy vehicles. The goal is to develop the ability to safely store and release sufficient natural gas at low pressure (<1000psi) to power an urban delivery van for 80 miles.

Keywords: Natural Gas Storage, Carbon Monolith

63. **IMPROVED MATERIALS FOR HEAVY VEHICLE FRICTION AND BRAKE APPLICATIONS**
$525,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of these activities is to investigate the nature of changes on surfaces of materials during braking, develop understanding of the role of friction films in braking, to evaluate advanced materials for heavy vehicle brake application, and to develop reliable, cost-effective, laboratory-scale friction tests to select and rank new materials and surface treatments for engine components.

Keywords: Brakes, Friction Materials, Friction Films

64. **HIGH CONDUCTIVITY CARBON FOAMS FOR THERMAL MANAGEMENT**
$125,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of this activity is to evaluate the use of conductive carbon foam materials as a highly efficient and lightweight heat exchanger for heavy vehicle cooling needs such as radiators, etc. Focus is on determining basic material properties, defining acceptable operating limits, and fabrication of the core structures which can operate in a class 7-8 vehicle.

Keywords: Carbon Foam, Heat Exchanger, Heavy Vehicle

65. **ADVANCED JOINING TECHNOLOGY DEVELOPMENT**
$820,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 375-4478
Laboratory Partners: ANL, ORNL, PNNL

The objective of this project is to develop cost-effective technologies for joining lightweight materials as well as dissimilar materials for use in heavy vehicle structures.

Keywords: Friction Stir Processing, Dissimilar Materials, Ultrasonic Joining

66. **DEVELOPMENT OF ADVANCED MATERIALS FOR HEAVY VEHICLE APPLICATIONS**
$975,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ANL, NIST, ORNL, PNNL
Industry Partners: Caterpillar, AFS
University Partners: Brown University, University of Virginia, Ohio State University

The objective of this project is to evaluate advanced lightweight materials and processes that can potentially reduce weight or enhance the performance and durability of heavy vehicles. Materials that are being considered include magnesium, titanium, metal matrix composites or carbon fiber-reinforced polymer composites, as well as non-conventional materials.

Keywords: Advanced Processes, Advanced Materials, Titanium, Magnesium, Mmc

67. **IMPLEMENTATION OF LIGHTWEIGHT MATERIALS IN HEAVY VEHCILE STRUCTURAL APPLICATIONS**
$2,175,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069, Dave Warren (865) 574-9693
PNNL Contact: Mark Smith (509) 375-4478
Laboratory Partners: ORNL, PNNL
Industry Partners: Freightliner, PACCAR, Delphi, Volvo, Heil Trailer, International Truck and Engine

The objective of this project is to develop cost-effective manufacturing processes and design procedures for metals and alloys and carbon fiber reinforced composite materials, alone, or together with lightweight metals, for applications aimed at reducing the mass of Class 8 trucks to improve fuel economy. Research efforts are concentrating on both body and frame members and emphasize the use of high performance fibers embedded into commodity grade resin systeMs. Component and subsystem mass reductions in excess of 50 percent are the goal of each research effort. Other efforts focus on innovative engineered materials.

Keywords: Carbon Fiber Reinforced Composites, Structural Components, Polymer Processing, Magnesium, Aluminum, Foamed Metals

68. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,700,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 375-4478
Laboratory Partners: ORNL, PNNL

The objective of these activities is: to provide assessment of various technologies, to conduct workshops to assess technology needs for the trucking industry, to develop multi-year program plans, and to provide guidance to program management as to appropriate investments for R&D funding, and to fund innovative research with small businesses.

Keywords: Cost, Planning, Workshops, Technical Management, Assessments

HIGH TEMPERATURE MATERIALS LABORATORY

69. **HIGH TEMPERATURE MATERIALS LABORATORY USER PROGRAM**
$5,600,000
DOE Contact: James Eberhardt (202) 586-9837
ORNL Contact: Arvid Pasto (865) 574-5123

The HTML (High Temperature Materials Laboratory) is a national user facility, offering opportunities for American industries, universities, and other federal agencies to perform in-depth characterization of advanced materials under the auspices of its User Program. Available are electron microscopy for microstructural and microchemical analysis, equipment for measurement of the thermophysical and mechanical properties of materials to elevated temperatures, X-ray and neutron diffraction for structure and residual stress analysis, high speed grinding machines, and measurement of component shape, tolerances, surface finish, and friction and wear properties.

Keywords: Materials Characterization, Ceramics, Composites, Alloys, Components

GEOTHERMAL TECHNOLOGIES PROGRAM

	FY 2003
GEOTHERMAL TECHNOLOGIES PROGRAM - GRAND TOTAL	$310,000
GEOTHERMAL MATERIALS	$310,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$310,000
Non-Destructive Testing and Piping Integrity Assessment	250,000
Structural Response Analysis for Well Cements	60,000

GEOTHERMAL TECHNOLOGIES PROGRAM

The primary goal of the geothermal materials program is to ensure that the private sector development of geothermal energy resources is not constrained by the availability of technologically and economically viable materials of construction. This requires the performance of intermediate and long-term high-risk materials research and development.

GEOTHERMAL MATERIALS

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

70. **NON-DESTRUCTIVE TESTING AND PIPING INTEGRITY ASSESSMENT**
$250,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M.L. Berndt (631) 344-3060 and
A.J. Philippacopoulos (631) 344-6090

The objective of this project is to evaluate methods for long-range non-destructive testing, integrity assessment and repair of geothermal piping systeMs. The research involves: a) evaluation of NDT methods as applied to specific problems encountered in geothermal piping with emphasis on on-line, long range techniques; b) integration of the results from NDT with remaining strength assessment; and c) development of in-situ repair/strengthening materials and methods.

The first part of the project has involved determination of the limitations of current practices used by the geothermal industry for assessing pipe condition and the desirable attributes of better inspection methods. From this information, alternative methods and the development of new methods have been considered. These investigations have led to delineation of ultrasonic guided wave testing as a potential global inspection technology suitable for long range detection of defects. This method will be field tested in FY04.

In the second area of the project, methodologies and the level of detail required from NDT for remaining strength assessment of geothermal piping are being investigated so that inspection and maintenance programs can be optimized. Existing analytical and numerical methods have been reviewed and a systematic approach for integrity assessment of internally corroded geothermal piping is being developed.

The third part of the project deals with in-situ repair/strengthening of geothermal piping systeMs. Composite wraps are being considered for this purpose. The work will involve experimental evaluation of the relevant material properties of candidate high temperature composites. It is also necessary to analyze the stresses in repaired corroded piping in support of determining suitability for repair and required properties and configuration of the repair material.

Keywords: Geothermal Piping, Non-Destructive Testing, Corrosion, Plant Reliability, Ultrasonics, Guided Waves

71. **STRUCTURAL RESPONSE ANALYSIS FOR WELL CEMENTS**
$60,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M.L. Berndt (631) 344-3060 and
A.J. Philippacopoulos (631) 344-6090

The objective of this program was to investigate the mechanical behavior of well cements using material testing confirmed by structural modeling of the response behavior of geothermal wells. These investigations address ways of improving the performance of geothermal wells through material characterization and modeling of well response due to pressure and temperature loads occurring in steady-state or transient forMs. Owing to reduced funding and work scope in FY03, research concentrated on characterization of well cements under tensile loads. Instrumentation necessary for performing direct tensile tests on well cements was developed. Different cement formulations were then tested to compare the tensile behaviour and then relate this to expected in-situ performance. The materials tested included conventional, latex-modified, fibre reinforced and lightweight formulations. The fibres studied were carbon microfibres, steel microfibres and steel macrofibres. Durability tests on steel fibre reinforced cements were performed to examine corrosion characteristics and determine whether tensile strength was maintained. Finally, the rate of strength development in fibre reinforced well cements was investigated.

Keywords: Geothermal Wells, Cements, Mechanical Behavior, Material Testing, Fiber Reinforcement, Structural Analysis

HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM

	FY 2003
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM - GRAND TOTAL	$6,527,500
HYDROGEN STORAGE MATERIALS PROGRAM	$5,535,000
Investigation of Catalytically Enhanced Complex Metal Hydride Materials for Hydrogen Storage	260,000
Hydride Development for Hydrogen Storage	1,875,000
High Density Hydrogen Storage System Prototype Using $NaALH_4$ Based Complex Compound Hydrides	1,250,000
Hydrogen Storage in Carbon Single-wall Nanotubes	2,150,000
FUEL CELL MATERIALS PROGRAM	$992,500
Microstructural Characterization of PEM Fuel Cells	200,000
Cost-Effective Metallic Bipolar Plates Through Innovative Control of Surface Chemistry	300,000
Compact Carbon Foam Radiator for Fuel Cell Power Systems	142,500
Selective Catalytic Oxidation of Hydrogen Sulfide	350,000

HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM

HYDROGEN STORAGE MATERIALS PROGRAM

72. **INVESTIGATION OF CATALYTICALLY ENHANCED COMPLEX METAL HYDRIDE MATERIALS FOR HYDROGEN STORAGE**
$260,000
DOE Contact: C. J. Read (202) 586-3152
University of Hawaii Principal Investigator: C. Jensen (808) 956-2769

The University of Hawaii is developing catalytically enhanced complex hydride storage materials capable of being used in vehicular applications. In particular, the objective of this research is to develop methods of doping sodium aluminum hydride, $NaAlH_4$, with titanium and/or zirconium that give rise to state-of-the-art hydrogen storage materials. This research has contributed to the state-of-the-art in enhancing the dehydrogenation (e.g., hydrogen discharge) and hydrogenation (e.g., hydrogen uptake) processes. However, it has not yet been demonstrated that ~5 weight percent hydrogen can be reversibly released from these materials under conditions that are required for the practical operation of an onboard fuel cell. Most notably, the kinetics and thermodynamics of the second dehydrogenation reaction remain impractical for hydride that is doped with titanium, and improved variations of this material must be produced to achieve commercial viability. To guide our development of advanced alanates, we have sought to gain a fundamental understanding of the nature of the dopants and the structural effects they exert on the hydride using novel material synthesis strategies and detailed structural and functional characterizations. The fundamental understanding gained from the alanate system can then be applied towards the design of other complex hydrides with higher capacities that have the potential of surpassing the DOE/FreedomCAR performance targets for on-board storage.

Keywords: Complex Hydrides, Alanates, Hydrogen Storage

73. **HYDRIDE DEVELOPMENT FOR HYDROGEN STORAGE**
$1,875,000
DOE Contact: C. J. Read (202) 586-3152
SNL Contact: J. Wang (925) 294-2786

The purpose of this project is to develop and demonstrate the next generation of practical hydrogen storage materials. This program focuses on complex metal hydrides with high reversible hydrogen storage capacities and novel approaches to on-board hydrogen storage systeMs. This research is based on achievements that Sandia has made in developing advanced Ti-doped Na alanates. The discovery of enhanced hydrogen sorption by Ti-doped alanates opened up an entirely new prospect for lightweight hydrogen storage. These materials have nearly ideal equilibrium thermodynamics, high capacities, and moderate kinetics. However, while the hydrogen capacity is 2 to 3 times better than commercial low-temperature hydrides, it does not meet the DOE/FreedomCAR storage capacity targets. Thus, other higher capacity reversible complex hydrides must be developed. At the same time, Na alanates continue to provide a good working model to better understand reversible hydrogen sorption in complex hydrides. Sandia's direct synthesis process and new Ti-doping methods have led to a dramatic improvement in the reversible hydrogen capacity and hydrogen absorption and desorption rates. These methods will be employed to seek out advanced complex hydrides with larger hydrogen storage capacities and better performance. Ti-doped Mg_2FeH_6 has been investigated as an analog to the alanate system. Using Sandia's direct synthesis and doping approach, it was found that Ti-halides (Cl, F, Br) all successfully enhance kinetics with $TiCl_2$ providing the best results. It was also determined that non-reactive precursors (TiH_2 and pre-reacted halides) improve kinetics, opening up new routes to improve capacity. Through collaborations with universities and other labs, we have performed in-depth NMR, neutron diffraction, and ESR measurements studies. These have aided in furthering our understanding of the Ti-doping mechanism. Pressure composition temperature isotherm measurements have been performed on Na alanate.
These measurements indicate that Ti-doping modifies the thermodynamic stability of the materials as well as the kinetics of hydrogen sorption.

Keywords: Complex Hydrides, Alanates, Hydrogen Storage

74. **HIGH DENSITY HYDROGEN STORAGE SYSTEM PROTOTYPE USING $NaAlH_4$ BASED COMPLEX COMPOUND HYDRIDES**
$1,250,000
DOE Contact: C. J. Read (202) 586-3152
United Technologies Research Center Contact: D. Anton (860) 610 7174

This project is focusing on the reversible complex hydride, $NaAlH_4$, with a theoretical hydrogen capacity of 5.5 wt%, and seeks to enhance the material for improved charging and discharging rates as well as increased hydrogen capacity. Safety studies of the enhanced material are continuing to support the technology as it is driven toward commercialization. The project also seeks to apply this material in the development of a prototype system which will reversibly store a high wt% of hydrogen at low pressure for an indefinite amount of time. The design of the system is also meant to be flexible towards using similar behaving complex hydrides in addition to sodium alanate. The storage system which contains the complex hydride powder must serve two primary functions: 1) exchange heat between the powder and a working liquid to drive the absorption/desorption of hydrogen; 2) support elevated hydrogen pressure during refueling. These functions must be performed with a minimum of weight, volume and cost. In addition, there are other secondary characteristics such as (i) allowing for significant volumetric change of the powder, (ii) exchanging hydrogen without the loss of the fine hydride powder particles, (iii) maintaining chemical compatibility with the hydride powder and hydrogen, (iv) producing minimal impurities going to the PEM fuel cell, and (v) fitting into a conformable volume. The project has included both materials development and system design. For the materials development, combined atomistic/thermodynamic models of the $NaAlH_4$ system were created to determine catalyzed compositional ranges, sorption mechanisms and the effects various catalyst additions have on these mechanisMs. The materials were then cyclically evaluated to determine degradation mechanisms and ameliorations as well as compatibility with construction materials. For the prototype storage system design and construction, standardized safety testing was conducted related to the classification of hazardous materials. Engineering design included performing heat and mass flow modeling for detailed optimization of the required system volume, mass and hydrogen sorption characteristics. Methods to enhance heat conduction into the metal hydride powder were evaluated. Currently, the 1-kg hydrogen storage system is under construction for testing in the near term.

Keywords: Complex Hydrides, Alanates, Hydrogen Storage System

75. **HYDROGEN STORAGE IN CARBON SINGLE-WALL NANOTUBES**
$2,150,000
DOE Contact: S. Satyapal (202)586-2336
NREL Contact: M.J. Heben (303)384-6641

The long-term goal of the project is to enable efficient adsorption of hydrogen at ambient temperature and pressure on nanostructured carbon materials. Of particular interest are the “engineered” nanostructured carbons such as carbon single-wall and multi-wall nanotubes (SWNTs and MWNTs), graphitic nanoparticles or cages, and conducting polymers. Graphite-encapsulated metals have been found to be more easily removed from crude SWNT materials if CO_2 oxidation is employed prior to the conventional purification process. Hot wire chemical vapor deposition (HWCVD) has been developed as a continuous and scaleable technique for the production of MWNTs at high density. HWCVD has also been demonstrated for continuous production of SWNTs. The presence of small quantities of transition metals has been shown to enhance the hydrogen adsorption capacities of graphitic materials. Metal-assisted hydrogen adsorption at near ambient conditions on carbon nanotubes only occurs when small metal nanoprticles are in intimate contact with the nanotubes. The evaporation of Pd instead of Ti onto carbon nanotube materials will likely be more effective in hydrogen adsorption catalysis, since Pd is not oxidized in air at room temperature. Both conducting carbon polymers and HWCVD-generated Fe-doped nanocarbons are promising candidates for hydrogen storage materials.

Keywords: Carbon Materials, Carbon Nanotubes, Hydrogen Storage

FUEL CELL MATERIALS PROGRAM

76. **MICROSTRUCTURAL CHARACTERIZATION OF PEM FUEL CELLS**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: T. R. Armstrong (865) 574-7996
ORNL Principal Investigator: K. L. More
(865) 574-7788

This goal of this project is to correlate the structural and compositional changes of PEM MEAs to electrochemical performance after testing under load. In addition, correlations will be drawn as to how the MEAs were processed. The technique for preparing ultrathin cross-sections of PEM fuel cell MEAs for characterization in a transmission electron microscope (TEM) has been previously developed and improved to the point where 100 nm thick sections are routinely achieved. These sections allow characterization of all of the important features of the MEA microstructure. Current studies are focused on evaluating the: 1) effect of recast Nafion content in catalyst layers, 2) effect of different electrocatalysts (Pt, PtRu, Pt_3Cr, PtCoCr), 3) effect of catalyst application technique, and 4) effect of H_2SO_4 boiling step. Structural changes after aging (operation under load) for up to 5,000 hrs are also being evaluated. Evaluation of samples provided by LANL has shown minor coarsening of the Pt_3Cr cathode catalyst and migration of the catalyst to the cathode/membrane interface. On the anode side, more severe coarsening of the catalyst was observed along with migration (potentially dissolution re-precipitation) of the Pt more than 3 mm into the membrane. Both of these occurrences were observed after 1000 hrs of cell operation. Future work encompasses completion of current work underway with LANL, Gore, Plug Power, and Fuel Cell Energy, to further improve the TEM preparation technique for gas diffusion layers, and initiate evaluation of Nafion for chemical or compositional changes using energy loss spectroscopy. These efforts involve collaborations with LANL, Gore, Plug Power, Fuel Cell Energy, and Battelle Memorial Institute.

Keywords: Transmission Electron Microscopy, MEA, Microstructure, Aging

77. **COST-EFFECTIVE METALLIC BIPOLAR PLATES THROUGH INNOVATIVE CONTROL OF SURFACE CHEMISTRY**
$300,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: T. R. Armstrong (865) 574-7996
ORNL Principal Investigator: M. P. Brady
(865) 574-5153

The goal of this effort is to develop a low cost metallic bipolar plate alloy that will form an electrically conductive and corrosion resistant nitride surface layer during thermal nitriding to enable its use in a PEM fuel cell environment. Proof-of-principle for this approach was demonstrated by long-term corrosion evaluation and single-cell fuel cell testing of a model Ni-50Cr alloy nitrided to form a protective Cr-nitride surface layer. A 4000 hr. corrosion test was carried out using the Los Alamos National Lab (LANL) corrosion test cell which uses 80 sulfuric acid solutions doped with 2 ppm F^- sparged with H_2 or air to represent PEM anode and cathode bipolar plate conditions, respectively. Levels of only 3.81 ppm cumulative Ni were measured in the anode face solutions and 0.08 ppm in the cathode over the course of the exposure. No Cr dissolution was observed. Interfacial contact resistance (ICR) measurements of the 4000 hr exposed coupon conducted at the National Renewable Energy Lab showed no increase in ICR relative to the as-nitrided Ni-50Cr, in the goal range of <20 mohm-cm^2 at loads of 100-150 N/cm^2. Single-cell fuel cell testing using 50 cm^2 active area plates of nitrided Ni-50Cr operated at 0.7V and 80°C for 1000 hr. showed promising behavior with no increase in interfacial resistance attributable to the nitrided plates and very low levels of metal ion contamination of the polymer membrane (0.01-0.3 x 10^{-6} g/cm^2). Current work is focused on more aggressive fuel cell test conditions with nitrided Ni-50Cr plates to establish the performance limits and optimize the Cr-nitride surface, and the formation of similar protective Cr-nitride surfaces on lower Cr, Ni(Fe) and Fe-base alloys to meet DOE cost goals. These efforts involve collaborations with LANL, NREL, and several fuel cell OEMs and end-users.

Keywords: Bipolar Plates, Coatings, Corrosion Resistance, Fuel Cells, Nitride

78. **COMPACT CARBON FOAM RADIATOR FOR FUEL CELL POWER SYSTEMS**
$142,500
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: T. R. Armstrong (865) 574-7996
ORNL Principal Investigator: E. Lara-Curizo
(865) 574-1749

The objective of this project is to develop and evaluate graphite-based heat exchangers for thermal management of fuel cells and fuel cell powered vehicles. In particular, graphite foams with improved permeability and lower-cost alternatives to graphite foams (fibers) will be developed to meet the efficiency, durability and cost requirements of fuel cells and fuel cell powered vehicles. A collaboration with researchers at the University of Western Ontario (Canada) focused on modeling the carbon foam to optimize the microstructural scale and geometrical features of permeable materials that provide maximum heat transfer and minimum pressure drop. This effort concluded that the thermal conductivity of the carbon is not as important to heat transfer as the pore size of the material. Using those model predictions as guidelines, graphite foams with various pore sizes and pore distributions are being synthesized to determine their heat transfer and properties and permeability. In parallel, 3-D woven fiber structures using different grades of graphite fibers radiators are being designed and fabricated. The type of fiber and its orientation in the woven structure will be selected to maximize heat transfer while minimizing cost. The geometrical features of the woven structure (e.g. weaving pattern) and their scale (e.g., spacing between fill and warp bundles) will be evaluated in the heat exchanger test bed constructed for the EERE DER Program.

Keywords: Carbon, Radiator, Heat Exchanger, Thermal Management

79. **SELECTIVE CATALYTIC OXIDATION OF HYDROGEN SULFIDE**
$350,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: T. R. Armstrong (865) 574-7996
ORNL Principal Investigator: V. Schwartz
(865) 576-6749

The objective of this work is to develop a carbon-based catalyst that reduces the sulfur levels of hydrogen gas streams to the ppb level through a reaction that involves the oxidation of H_2S to elemental sulfur. Proof-of-principle for this approach was demonstrated by long-term evaluation of an ORNL derived carbon catalyst that, when operated at 150 , reduced 1000 ppm H_2S to less than 200 ppb without formation of unwanted oxidation products (COS or SO_2). Additional studies have shown that the activity of this catalyst is directly related to the internal pore size and volume and the concentration of basic surface reaction sites. The main failure mechanism is fouling of the pores with elemental sulfur. However, these catalysts can easily be regenerated by heating to 200 in air and then reused without any change in activity. The current generation of catalyst can reduce sulfur levels to less than 200 ppm for more than 40 days without regeneration. This catalyst has also demonstrated an affinity for removing COS from hydrogen containing gas streaMs. Current work is focused on determining the interrelationships between catalyst morphology, surface functional groups and charge, and catalyst chemistry on activity and durability. The durability of the catalysts will be investigated and a regeneration protocol improved. These efforts involve collaborations with NETL and discussions are underway to expand the collaborators to include ChevronTexaco and ConocoPhillips.

Keywords: Carbon Catalyst, Sulfur Removal, Fuel Processing

INDUSTRIAL TECHNOLOGIES PROGRAM

	FY 2003
INDUSTRIAL TECHNOLOGIES PROGRAM - GRAND TOTAL	$22,834,600
ALUMINUM SUBPROGRAM	$5,951,600
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$3,244,129
Inert Metal Anode Life in Low Temperature Aluminum Reduction Process	800,000
Intelligent Potroom Operation	152,675
Potlining Additives	284,778
Reduction of Oxidative Melt Loss of Aluminum	228,740
Selective Adsorption of Salts from Molten Aluminum	59,390
Aluminum Carbothermic Technology	1,200,000
High Efficiency Low Dross Combustion System	360,000
A Bubble Probe for Optimization of Bubble Distribution and Minimization of Splashing/ Droplet Formation	83,937
Microwave Assisted Electrolytic Cell	74,609
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,172,320
Reduction of Annealing Times for Energy Conservation in Aluminum Processing	80,000
Surface Behavior of Aluminum Alloys Deformed under Various Processing Conditions	85,124
Fundamental Studies of Structural Factors Affecting the Formability of Continuous Cast Aluminum Alloys	100,000
Development of a Two-phase Model for the Hot Deformation of Highly-Alloyed Aluminum	100,000
Development of Integrated Methodology for Thermo-mechanical Processing of Aluminum Alloys	110,787
Numerical Modeling of Transient Melt Flows and Interface Instability in Aluminum Reduction Cells	27,034
Low Temperature Reduction of Alumina Using Fluorine Containing Ionic Liquids	76,678
Effect of Impurities on the Processing of Aluminum Alloys in Casting, Extrusion, and Rolling	77,697
Combined Experimental and Computational Approach for the Design of Mold Surface Topography	72,000
Molten Aluminum Treatment by Salt Fluxing with Low Environmental Emissions	79,000
Inert Metal Anodes for Primary Aluminum Production	100,000
Improved Energy Efficiency in Aluminum Melting	190,000
Evaluation and Characterization of In-Line Annealed Continuous Cast Aluminum Sheet	74,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,535,151
Spray Rolling Aluminum Strip	150,436
Modeling Optimization of Direct Chill Casting	253,773
Degassing of Aluminum Alloys Using Ultrasonic Vibrations	40,000
Effect of Casting Conditions & Composition on Microstructural Gradients in Roll Cast Aluminum Alloys	66,906
Energy Efficient Isothermal Melting of Aluminum	400,000
Coolant Characteristics and Control in Direct Chill Casting of Aluminum	40,036
Continuous Severe Deformation Processing of Aluminum Alloys	384,000
Development of a Rolling Process Design Tool for Use in Improving Hot Roll Slab Recovery	200,000
GLASS SUBPROGRAM	$200,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$200,000
Development of Models and On-Line Diagnostic Monitors of the High-Temperature Corrosion of Refractories in Oxy-Fuel Glass Furnaces	200,000

	FY 2003
METAL CASTING SUBPROGRAM	$1,279,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$473,000
Creep Resistant Zinc Alloy Development	132,000
Development of Surface Engineered Coatings for Die Casting Dies	244,000
Integration of RSP Tooling with Rapid Prototyping for Die-Casting Application	97,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING	$806,000
Clean Cast Steel: 1) Machinability of Cast Steel; 2) Accelerated Transfer of Clean Steel Technology	98,000
Prevention of Porosity in Iron Castings	25,000
Advanced Lost Foam Casting Technology	180,000
Metallic Reinforcement of Direct Squeeze Die Cast Aluminum Alloys	100,000
Ferrite Measurements in Duplex Stainless Steel Castings	120,000
Technology for the Production of Clean, Thin Wall, Machinable Gray and Ductile Iron Castings	77,000
Improvements in Sand Mold/Core Technology: Effects on Casting Finish	106,000
Heat Checking and Washout of Superalloys for Die Inserts	100,000
STEEL SUBPROGRAM	$3,468,000[7]
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,681,758
Controlled Thermo-mechanical Processing of Tubes and Pipes for Enhanced Manufacturing and Performance	1,983,250
Life Improvement of Pot Hardware in Continuous Hot Dipping Processes	450,000
Plant Trial of Non-Chromium Passivation Systems for Electrolytic Tin Plate	248,508
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,929,189
Research Related to the Development of the Automated Steel Cleanliness Analysis Tool (ASCAT)	300,000
Enhanced Inclusion Removal from Steel in the Tundish	813,045
Reducing the Variability of HSLA Sheet Steels	548,168
Constitutive Behavior of High Strength Multiphase Sheet Steels under High Strain Rate Deformation	1,023,060
Clean Steel – Advancing the State of the Art	421,612
Characterization of Formability of Advanced High Strength Steels	1,007,959
Development of a Standard Methodology for Quantitative Measurement of Steel Phase Transformation Kinetics and Dilation Strains Using Dilatometric Methods	1,152,348

[7]For every project within the American Iron and Steel Institute's (AISIs) Technology Program Roadmap Program (TRP), the funding shown is the total over the life of the project. Total DOE/ITP TRP funding in FY03 was $3,468,000.

INDUSTRIAL TECHNOLOGIES PROGRAM

	FY 2003
STEEL SUBPROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
Characterization of Fatigue and Stress/strain Behavior in Advanced High Strength Steels	385,221
Validation of Hot Strip Mill Model	2,594,476
Inclusion Optimization for New Generation Steel Products	448,210
Development of Appropriate Spot Welding Practice for Advanced High Strength Steels	235,090
MATERIALS PREPARATION, SYNTHESIS DEPOSITION, GROWTH OR FORMING	$4,418,540
Ironmaking Challenge – the Mesabi Nugget Research Project	3,596,540
Development of Steel Foam Materials and Structures	822,000
MATERIALS SUBPROGRAM	$11,936,000
DEGRADATION RESISTANT MATERIALS	$11,936,000
COATINGS AND SURFACE MODIFICATIONS	$1,585,000
Advanced Composite Coatings for Industries of the Future	660,000
Development of Ultrananocrystalline Diamond (UNCD) Coatings for SiC Multipurpose Mechanical Pump Seals	500,000
High Density Infrared (HDI) Transient Liquid Coatings (TLC) for Improved Wear and Corrosion Resistance	300,000
High Energy Density Coating of High Temperature Advanced Materials for Energy Efficient Performance	125,000
MATERIALS DEVELOPMENT AND PROCESSES	$4,856,403
Advanced Nanoporous Composite Materials for Industrial Heat Applications	300,000
Crosscutting Industrial Applications of a New Class of Ultra-Hard Borides	2,866,403
Development of a New Class of Fe-3Cr-W (V) Ferritic Steels for Industrial Process Applications	375,000
Development of Stronger and More Reliable Cast Austenitic Stainless Steels (H-series) Based on Scientific Design Methodology	175,000
Exploring Ultrahigh Magnetic Field Processing of Materials for Developing Customized Microstructures and Enhanced Performance	200,000
Novel Superhard Materials and Nanostructured Diamond Composites for Multiple Industrial Applications	716,000
Ultrasonic Processing of Materials	100,000
Fracture Toughness and Strength in a New Class of Bainitic Chromium-tungsten Steels	124,000
REFRACTORIES	$500,000
Development of Cost Effective Ceramic and Refractory Components for Aluminum Melting and Casting	300,000
High Density Infrared Treatment of Refractories	200,000

INDUSTRIAL TECHNOLOGIES PROGRAM

	FY 2003
INDUSTRIAL MATERIALS FOR THE FUTURE (continued)	
DEGRADATION RESISTANT MATERIALS (continued)	
DATABASES AND MODELING	$1,400,000
Thermochemical Models and Databases for High Temperature Materials Processing and Corrosion	1,000,000
Development of Combinatorial Methods for Alloy Design and Optimization	200,000
Inverse Process Analysis for the Acquisition of Thermophysical Property Data	200,000
MATERIALS FOR SEPARATIONS	$218,295
Novel Modified Zeolites for Energy-efficient Hydrocarbon Separations	218,295
MATERIALS FOR ENGINEERING COMPONENTS	$2,026,302
Advanced Chlor-Alkali Technology	600,000
Development and Demonstration of Advanced Tooling Alloys for Molds and Dies	480,000
Stress-Assisted Corrosion in Boiler Tubes	276,000
Virtual Welded-Joint Design Integrating Advanced Materials and Processing Technologies	100,000
High-performance, Oxide-Dispersion-Strengthened Tubes for Production of Ethylene and Other Industrial Chemicals	185,278
Novel Carbon Films for next Generation Rotating Equipment Applications	209,709
Physical and Numerical Analysis of Extrusion Process for Production of Bi-Metallic Tubes	175,315
OTHER	$1,350,000
Metals Processing Laboratory Users (MPLUS) Facility	1,350,000

INDUSTRIAL TECHNOLOGIES PROGRAM

ALUMINUM SUBPROGRAM
The DOE Aluminum Team leader is Tom Robinson
(202) 586-0139

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

80. **INERT METAL ANODE LIFE IN LOW TEMPERATURE ALUMINUM REDUCTION PROCESS**
$800,000
DOE Contact: Tom Robinson (202) 586-0139

Northwest Aluminum Technologies and Brooks Rand, Ltd. are project partners for the development of this technology. A carbon-free aluminum reduction process is being developed as a modification to the Hall-Héroult process for primary aluminum production. The process uses a non-consumable metal alloy anode, a wetted cathode, and an electrolytic bath, which is kept saturated with alumina at the relatively low temperature of 750°C by means of free alumina particles suspended in the bath. In conducting the research, two primary tasks are involved. First, laboratory scale cells will be operated to firmly establish the viability of the fundamental concepts required for a successful commercial process. Second, a pilot scale 5000-ampere cell will be designed, constructed and operated. This task will address engineering aspects associated with scaling, such as liner fabrication, electrode configuration and design, and bath composition adjustments. This technology, once developed, will produce primary aluminum metal with lower energy intensity, lower cost, and lower environmental degradation than the conventional process.

Keywords: Aluminum Reduction, Inert Metal Anode, Smelting, Alumina Crucible Cell, Voltage

81. **INTELLIGENT POTROOM OPERATION**
$152,675
DOE Contact: Tom Robinson (202) 586-0139

Applied Industrial Solutions, Century Aluminum, and West Virginia University are project partners for the development of intelligent potroom operation. Aluminum smelting requires operators to oversee many refining cells. Scrutiny of each one on a regular basis is not possible. In addition, modern aluminum refining cell controllers attempt to optimize cell efficiency by controlling the concentration of alumina in the bath. Unfortunately, no direct measure of alumina concentration is yet possible. The ramifications miscalculating alumina concentration is significant from an environmental and energy efficiency standpoint. One major product of this research will be the development of a Corrective Action Neural Network (CANN). Its function is to monitor and analyze data from the pots on a continuous basis, looking for cells whose performance is deteriorating. It will anticipate which cells are about to slip into degraded or out-of-control operation and dispatch the operator to intervene before trouble begins. Eventually, a closed-loop Cell Control Enhancement Module (CCEM) will be added to the individual cell controllers. The CCEM will use an enhanced instrumentation package and powerful data analysis techniques to provide a more complete picture of instantaneous cell status to the CANN. The CANN and CCEM will work in concert to continuously improve the database on each cell, and the knowledge base on control and remediation techniques.

Keywords: Smelting, Aluminum Potroom Operation, Aluminum Refining

82. **POTLINING ADDITIVES**
$284,778
DOE Contact: Tom Robinson (202) 586-0139

This project is designed to further examine the potential benefits derived from the addition of boron oxide to potlining used in primary aluminum production cells. A relatively inexpensive bulk chemical, boron oxide not only suppresses cyanide formation, but also may inhibit sodium intercalation and, above all, promote, in the presence of some titanium, wetting of cathode carbonaceous material by the metal pad, thus reducing ohmic cell resistance and sludge formation. Improvements in energy consumption, waste disposal and overall economics of the process are projected. Laboratory testing and commercial scale testing will investigate parameters that are important for the commercial application. Tests in industrial cells will complement laboratory testing. Carbonaceous potlining components added with boron oxide will be incorporated in industrial cells in later phases of the program, providing results of the first year are positive. Project partners include Century Aluminum of West Virginia, Inc., EMEC Consultants, the NSA Division of Southwire Company and SGL Carbon Corporation.

Keywords: Potlining, Smelting, Aluminum Production, Boron Oxide, Aluminum Production Cells

83. **REDUCTION OF OXIDATIVE MELT LOSS OF ALUMINUM**
$228,740
DOE Contact: Tom Robinson (202) 586-0139

Fabrication of virtually all finished aluminum products requires melting. During the melting process, an average of 4 percent of the input material is lost to oxidation. The lost material takes three forms in the furnace: 1) dross, a mixture of aluminum oxide compounds and aluminum metal typically skimmed from the surface of the melt; 2) inclusions entrained in the molten metal removed by filtration; and 3) oxide sludge found at the bottom of the melt. In the U.S., an annual energy loss of approximately 70 trillion Btu results from oxidative melt loss of over 960 million pounds of aluminum. This project will target practices to significantly reduce these losses. The melt loss project will identify aluminum melting practices that will increase energy efficiency and decrease material losses. The project will lower the cost of aluminum products, reduce energy consumption, reduce industrial emissions, and significantly increase the recycling capability of the aluminum industry. An increased fundamental understanding of the oxidation of molten aluminum will be developed to be a cross-section of the aluminum industry. Project partners include Secat, Inc., Commonwealth Aluminum, Hydro Aluminum, IMCO Recycling Inc., NSA Division of Southwire Co., Alcan Aluminum Corp., ARCO Aluminum Inc., McCook Metals LLC, Albany Research Co., Argonne National Laboratory, Oak Ridge National Laboratory, and University of Kentucky.

Keywords: Dross, Aluminum Melting, Oxide Sludge

84. **SELECTIVE ADSORPTION OF SALTS FROM MOLTEN ALUMINUM**
$59,390
DOE Contact: Tom Robinson (202) 586-0139

Selee Corp. and Alcoa are project partners for the development of this Selective Adsorption technology. Primary aluminum is produced by the reduction of alumina in electrolytic cells. Cells contain a molten cryolite bath in which the alumina is dissolved. When an electric current is applied, aluminum is released and settles to the bottom of the cell. Molten aluminum is withdrawn to holding furnaces, and alumina is added to the bath as it is consumed. In normal production, a small portion of the bath is carried over with the molten aluminum. Most of the bath carry-over can be removed by careful skimming and good transfer practices. However, some carry-over of the bath to the metal holding furnace is common. Cryolite bath contains sodium and small amounts of calcium and lithium. These metal salts must be removed from aluminum in the holding furnace to produce metal of commercial value. Chlorine is used to remove these salts. Bath carry-over is undesirable because it adds significantly to the time required and the amount of chlorine used to make commercial aluminum. A new microporous material has been demonstrated to selectively adsorb salts from molten aluminum in holding furnace operations. This project will evaluate the potential of adapting these microporous materials to remove carry-over salts. Successful removal of these salts will result in significant reductions of energy, chlorine and metal loss.

Keywords: Alumina, Microporous Materials, Cryolite, Primary Aluminum

85. **ALUMINUM CARBOTHERMIC TECHNOLOGY**
$1,200,000
DOE Contact: Tom Robinson (202) 586-0139

Alcoa Technical Center, Elkem Aluminum Division, and Carnegie Mellon University are project partners for the development of the advanced reactor process (ARP). ARP is a new process for the production of aluminum by carbothermic reduction. This technology has been proposed as an alternative to the current Hall-Héroult electrolytic reduction process. ARP has the potential to produce primary aluminum at a power consumption in the range of 8.5 kWh/kg at an estimated 25 percent reduction in manufacturing cost. Although the carbothermic process involves the generation of carbon-based greenhouse gases (GHG), the total GHG reduction from power plant to metal should be substantial due to the significantly reduced power consumption, the elimination of perfluorocarbon emissions, and the elimination of carbon anode baking furnace emissions. The estimated capital investment required for ARP will be about 50 percent less than that for Hall-Héroult cell technology. The labor required for plant operation will also be reduced. ARP is a multi-step high temperature chemical reaction that produces aluminum by reduction of alumina with carbon. Optimization for reaction products requires a multi-zone furnace operating at temperatures in excess of 2,000°C. A significant portion of the aluminum is in the gas phase at these temperatures. A continuously operating furnace capable of producing the high temperatures required and recovering the molten and gas phase products is critical for the development of this technology. This is Phase I of a multi-phase effort to develop an ACT reactor based on advanced, high temperature, electric-arc furnace technology and improved understanding of the process reactions.

Keywords: Aluminum Carbothermic Reduction, Advanced Reactor Process, Alumina

86. **HIGH EFFICIENCY LOW DROSS COMBUSTION SYSTEM**
$360,000
DOE Contact: Tom Robinson (202) 586-0139

Over 70 percent of 2.3 million tons of secondary aluminum recovered from scrap is processed in reverberatory furnaces. These furnaces are widely used because of their versatility and low capital cost. Despite their benefits, reverberatory furnaces exhibit uneven surface temperature and exposure to oxygen that promotes the production of dross on the surface of the molten aluminum. Dross formation lowers aluminum productivity and insulates the molten aluminum thereby lowering energy efficiency. This project will develop and demonstrate a high-efficiency low-dross combustion system for secondary aluminum natural gas-fired reverberatory furnaces. Oxygen enrichment is key to improving burner efficiency and has been demonstrated in many industries. Oxygen enriched flames are hotter than air-fired flames and can promote dross formation. However, new burners and controls allow for the control of the flame shape and distribution of oxygen within the flame. Controlling the flame with a fuel rich zone on the flame bottom ensures that the molten aluminum has minimal exposure to oxygen and minimizes dross formation. At the same time, control of the flame shape ensures that the surface is evenly heated. Upon successful completion, this project will decrease energy requirements, improve economics, and decrease gaseous and solid emissions from the remelting of aluminum. This technology can also be retrofitted to existing reverberatory furnaces. Project partners include Gas Technology Institute, assisted by Wabash Alloys, LLC, Eclipse Combustion Inc., and University of Illinois Chicago.

Keywords: Reverberatory Furnace, Low-Dross Combustion, Secondary Aluminum

87. **A BUBBLE PROBE FOR OPTIMIZATION OF BUBBLE DISTRIBUTION AND MINIMIZATION OF SPLASHING/ DROPLET FORMATION**
$83,937
DOE Contact: Tom Robinson (202) 586-0139

Primary and secondary aluminum producers and foundries remove impurities from molten aluminum by bubbling chlorine through the molten metal as a reactive fluxing gas. An example of chlorine fluxing is the removal of magnesium from close to 64 billion recycled aluminum cans (2 billion pounds of aluminum) to match the high purity that is representative of aluminum produced from electrolytic cells. Primary aluminum producers also use gas fluxing to remove trace alkali metals from the electrolyte present in the electrolytic cells. However, fluxing yields toxic gases such as hydrogen chloride and chlorine as well as aluminum oxide fumes. Chlorine bubbling is poorly controlled. Excess chlorine is used to ensure impurities are reduced to acceptable levels, which results in both the loss of aluminum (AlCl3) and the emission of oxide fumes and toxic gases. Optimizing fluxing gas bubble size, frequency and residence time, and understanding how gas throughput may be increased without splashing and spraying of molten metal as the bubbles burst at surface would substantially reduce chlorine usage, increase productivity and thermal efficiency of aluminum purification process, and reduce toxic gas emissions. Project partners include University of California, Berkeley, assisted by Alcoa Technical Center.

Keywords: Gas Fluxing, Chlorine, Primary Aluminum

88. **MICROWAVE ASSISTED ELECTROLYTIC CELL**
$74,609
DOE Contact: Tom Robinson (202) 586-0139

This research is to develop a new electrometallurgical technology by introducing microwave radiation into the electrolytic cells for primary aluminum production. Michigan Technological University, collaborating with Cober Electronic, Inc. and Century Aluminum Company will provide technical, economic, and energy data for evaluation of this technology by conducting bench-scale research. Controlling alumina solubility in the electrolyte is critical for low temperature operations. The proposed technology takes advantage of the microwave capability of increasing alumina solubility kinetics, so the reaction can occur at lower operating temperature. The lower operation temperature provides the possibility to use a nickel-based superalloy for manufacturing the inert anode and wetted cathode. The nickel-based superalloy is inert to oxidation at 750˚ C, wetted with molten aluminum, and has excellent salt corrosion resistance. The goal is to demonstrate the potential to enhance the electrolytic bath kinetics with microwave radiation to allow the use of materials that have demonstrated good electrolytic inertness at lower temperatures.

Keywords: Alumina, Electrometallurgical, Microwave, Electrolytic Cells, Primary Aluminum

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

89. **REDUCTION OF ANNEALING TIMES FOR ENERGY CONSERVATION IN ALUMINUM PROCESSING**
$80,000
DOE Contact: Tom Robinson (202) 586-0139

Annealing processes, in the early stages of aluminum processing, affect the structure and properties of the material. A necessary step in processing all direct chill ingots is breakdown and hot rolling. In the typical single-stand mill, the time, temperature and deformation experienced by material varies considerably and is highly variable with respect to location along the work piece and across the section. Several large-volume, non-heat treatable aluminum alloys require one or more annealing steps in order to recrystallize the material. Recrystallization requires long-range motion of grain boundaries to restore the mechanical state ready for further processing, or sale to customer. Although recrystallization is a well understood process, very little is known quantitatively about the influence of impurities and crystallography on the critical process. The focus of this research will be to measure these effects, relate them to the actual compositions and deformation processing of real alloys and seek to minimize annealing times. Project partners will research how the annealing processes in early stages of aluminum processing affect the structure and properties of the material. Annealing at high temperatures consume significant amounts of time and energy. By making detailed measurements of the crystallography and morphology of internal structural changes, they expect to shorten processing times and use less energy during annealing while improving texture control in production of plate and sheet through a study of the kinetics of recrystallization in hot rolling. The research will exploit newly developed tools for textural and microstructural characterization to measure recrystallization kinetics and texture evolution. Project partners include Carnegie Mellon University, assisted by Alcoa Technical Center and the Pennsylvania Technology Investment Authority.

Keywords: Annealing, Recrystallization, Hot Rolling

90. **SURFACE BEHAVIOR OF ALUMINUM ALLOYS DEFORMED UNDER VARIOUS PROCESSING CONDITIONS**
$85,124
DOE Contact: Tom Robinson (202) 586-0139

Lehigh University and Alcoa Technology are project partners for establishing a relationship between surface behavior, metallurgy, and mechanical forming process parameters. Research will determine the fundamentals controlling surface microstructure development for rolling and extrusion processes. The objective is to understand the origins and mechanisms of the formation of surface phenomena including surface re-crystallization and surface fracture. Understanding the origins and mechanisms that control surface quality in formed aluminum products can help industry to reduce scrap, improve process efficiency, lower production costs, and save energy. Formed products are produced by complex thermo-mechanical deformation operations such as rolling and extrusion. These metal-forming operations can create surface flaws which affect surface anodizing and coating. Demand is rapidly growing for high quality formed aluminum products in the automotive and aerospace industries. Surface quality is part of the formed aluminum product specifications and is of comparable importance to mechanical properties and alloy composition.

Keywords: Surface Behavior, Metallurgy, Aluminum Alloys

91. **FUNDAMENTAL STUDIES OF STRUCTURAL FACTORS AFFECTING THE FORMABILITY OF CONTINUOUS CAST ALUMINUM ALLOYS**
$100,000
DOE Contact: Tom Robinson (202) 586-0139

University of Kentucky is collaborating with Commonwealth Aluminum Company, Oak Ridge National Laboratory, and Secat, Incorporated in conducting these studies. Aluminum sheets made by continuous casting (CC) provide an energy savings of at least 25 percent and an economic savings of more than 14 percent over sheets made from direct chill (DC) cast ingots. Width and formability are among the most important characteristics of aluminum sheets. There are substantial differences in the microstructures of CC and DC cast sheets that are a result of the casting process. Understanding the microstructure differences and how these relate to product forming is required before industry will invest the large capital required for wide continuous cast sheet equipment. The ability to continuously cast wide sheets with good formability microstructure will make the energy and economic savings available to a greater portion of the sheet forming market. The research will focus on determining the influence of the cast microstructure and the spatial distribution of the intermetallic constituents and dispersion phases of the microtexture during deformation and recrystallization. The object of this research is to study in detail the difference in structure between DC and CC aluminum alloys that leads to the difference in formability. This work will concentrate on the 5000 series aluminum alloys, which have great potential for continuous cast product market growth. The difference in formability will be correlated with the difference in bulk texture and microtexture of the two materials. The fundamental insight obtained from this research will provide a science-based approach for optimizing wide continuous casting technology.

Keywords: Continuous Casting, Microtexture, Direct Chill Casting

92. **DEVELOPMENT OF A TWO-PHASE MODEL FOR THE HOT DEFORMATION OF HIGHLY-ALLOYED ALUMINUM**
$100,000
DOE Contact: Tom Robinson (202) 586-0139

Conventional processing methods for highly alloyed aluminum consist of ingot casting, followed by hot rolling. These alloys are susceptible to the development of defects in hot rolling, due to localized melting along the chemistry rich grain boundaries. Much energy is wasted through the need to re-melt and reprocess. For both conventional hot rolling an novel processes such as continuous casting, quality will be achieved only through understanding of the flow of the alloyed aluminum at temperatures approaching the melting point. The research partners; University of Illinois, Alcoa, and Los Alamos National Laboratory, are developing a fundamental understanding for deformation of wrought alloys with emphasis on high temperatures bounding the hot working regime. Traditional constitutive models consider the alloy as a single-phase system. This research is offering a plan that spans the identification of fundamental deformation mechanisms using high-resolution electron microscopy and actualization into modeling capability appropriate for industrial processes. This research is developing a two-phase mathematical description for the high temperature flow of aluminum alloys. The focus is on hot rolling and provides a computation platform for optimization of the Thermo-mechanical processing window (TPW) within industrial capabilities of temperature and deformation rate. The key research challenge is the formulation of robust relations that detail mechanical behavior in the presence of a semi-solid phase. Success in the research effort and subsequent implementation in the domestic aluminum industry would provide an energy savings, a carbon dioxide reduction, a cost savings to the U.S. aluminum industry, and a reduction in scrap.

Keywords: Ingot Casting, Hot Rolling, Aluminum Alloys

93. **DEVELOPMENT OF INTEGRATED METHODOLOGY FOR THERMO-MECHANICAL PROCESSING OF ALUMINUM ALLOYS**
$110,787
DOE Contact: Tom Robinson (202) 586-0139

Washington State University, Alcoa Technology, and Pacific Northwest National Laboratory are project partners for the development of the integrated methodology for thermomechanical processing of aluminum alloys. The objective of this research is to develop an integrated methodology for modeling local structural evolution during thermomechanical processing (TMP) of rolled aluminum sheet for alloy design and manufacturing. Current alloys and processes are over-engineered at a substantial energy and material cost to aluminum producers. Better understanding of the physics of deformation and structure development will result in the opportunity to reduce alloy content, minimize processing steps, and improve performance of existing products. This research will involve developing a finite element based integrated mechanical and micro-structural model for process understanding and design sensitivity analyses and validating the integrated model predictions through bench-scale experimental measurements. The ultimate goal is to produce models that will allow simultaneous process modeling and alloy development. The integrated model will enable researchers to simultaneously address both materials dynamics and mechanical behavior for alloy design and for thermomechanical process optimization. The end-result will be processes optimized to reduce or eliminate energy intensive batch anneals during processing of automotive sheet. The integrated model will involve both local scale simulation of dislocation dynamics and microstructure evolution and macro-scale mechanical deformation simulations. The fundamental understanding and technology improvements derived from this research will translate into significant energy savings and great financial and environmental benefits to the aluminum industry.

Keywords: Thermomechanical Processing, Advanced Reactor Process, Alloys

94. **NUMERICAL MODELING OF TRANSIENT MELT FLOWS AND INTERFACE INSTABILITY IN ALUMINUM REDUCTION CELLS**
$27,034
DOE Contact: Tom Robinson (202) 586-0139

A key determinant in the energy consumption of aluminum smelting pots is the magnetohydrodynamic (MHD) stability of the metal pad/electrolyte interface. More stable designs permit operation at lower anode-to-cathode spacing, thus decreasing power consumption. More stable MHD designs also control anode effects which contribute to lost productivity and release of fluorine-based greenhouse gases. Incorporating new knowledge to allow better control of MHD effects in existing and design retrofit plants in the domestic smelting industry would decrease energy consumption. This research addresses the MHD induced melt flow and interface instabilities in aluminum reduction cells. The goal is to develop a tool useful for the analysis of MHD instabilities in smelting cells and then use it to gain understanding of the origin and nature of the MHD instabilities. The partners will develop an accurate and computationally efficient mathematical model that will incorporate substantially more relevant physics than the existing models. In particular, the melt flows and interface instability will be treated as coupled nonlinear nonsteady processes. An accurate mathematical model will help to achieve more stable design of the reduction smelters. This will allow lowering the anode-to-cathode distance, thus reducing the energy consumption.

Keywords: Magnetohydrodynamic, Smelting, Alloys, Anode, Cathode

95. **LOW-TEMPERATURE REDUCTION OF ALUMINA USING FLUORINE CONTAINING IONIC LIQUIDS**
$76,678
DOE Contact: Tom Robinson (202) 586-0139

No suitable substitute has been found for cryolite as a molten salt for the electrolytic reduction of aluminum, despite its high melting point. Cryolite's ability to dissolve alumina and its strong electrical conductivity has made it an inseparable part of the production of aluminum for the past 100 years. However, recently developed ionic liquids provide a new promising possibility for aluminum production. Ionic liquids are salts that are fluid at room temperature. Chloride ionic liquids have already shown the feasibility of reducing aluminum chlorides and fluoride-based ionic liquids can potentially be used to dissolve and reduce alumina at room temperature. Research partners will investigate the potential for using ionic liquids as the electrolytes for the production of primary aluminum. The research will focus on identifying a suitable ionic liquid that can be used for industrial electrodeposition of aluminum at temperatures significantly lower than those encountered in the Hall-Héroult process. The effect and optimization of the main electrolytic parameters will be studied, and the results will be compared with current technology. The fundamental insight obtained from this research will provide a science-based foundation for developing a process to produce aluminum at low temperatures, thus increasing energy savings and lowering costs.

Keywords: Cryolite, Electrolytic Reduction, Ionic Liquid, Hall-Héroult Process

96. **EFFECT OF IMPURITIES ON THE PROCESSING OF ALUMINUM ALLOYS**
$77,697
DOE Contact: Tom Robinson (202) 586-0139

Calcium, lithium and sodium are elements that are regarded as impurities in many aluminum alloys. The impurities contribute to the rejection rate of aluminum sheet and bar products. Rejected products must be remelted and recast. When products are remelted and recast, a portion of the aluminum is lost to oxidation (melt loss). Removal of these elements increases overall melt loss of aluminum alloys. Project partners are investigating the effect of impurities on the processing of aluminum alloys with the aim of lower product rejection rates with the resultant effect of lower melt losses. The goal of this project is to quantify the effect of impurities on the processing of multi-component aluminum alloys used in casting, extrusion, and rolling processes. Specific activities include: 1) development of thermodynamic data base on aluminum alloys containing Al, Na, Ca, Mg, and Li; 2) conduct computational thermodynamic simulations to determine the phase equilibria of multi-component alloys containing the impurity elements; 3) conduct kinetic simulations to determine the segregation behavior of the impurity elements and their influence on the phase evolution during processing conditions; and 4) verification of results of simulations by conducting experiments under industrial processing conditions.

Keywords: Alloys, Casting, Extrusion, Rolling, Thermodynamic, Oxidation, Melt Loss

97. **COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACH FOR THE DESIGN OF MOLD SURFACE TOPOGRAPHY**
$72,000
DOE Contact: Tom Robinson (202) 586-0139

One of the most challenging problems associated with metal casting is the control of heat extraction through the mold-shell interface during the early stages of solidification. This initial structure critically defines the downstream performance of the cast product. This experimental and computational effort is focused on investigating the effects of mold surface topography as well as of the physical and thermal properties of the mold (such as wettability of molten aluminum over the mold surface) on the geometric and physicochemical structure of the solidifying shell surface of aluminum castings. The work will integrate heat transfer and deformation analysis; melt flow, contact modeling (tribology) as well as metallurgical engineering. Finite element techniques will be used to model the ingot surface growth and inverse techniques will be employed to design the mold surface topographies that lead to desired morphologies at the freezing front surface. The mold surfaces will be characterized in terms of groove taper, depth, pitch and land roughness.

Keywords: Mold Surface Topography, Casting, Melt Flow, Tribology

98. **MOLTEN ALUMINUM TREATMENT BY SALT FLUXING WITH LOW ENVIRONMENTAL EMISSIONS**
$79,000
DOE Contact: Tom Robinson (202) 586-0139

Primary and secondary molten aluminum processing and refining involve fluxing metal with either pure chlorine gas or chlorine and inert gas mixture. The stack emissions caused by this gas injection include dust particles, hydrogen chloride, chlorine, and aluminum chloride gases. This research will investigate, understand, and minimize the emissions resulting from solid chloride flux addition to molten metal for alkali impurity and nonmetallic inclusion removal. Ohio State University will study the salt metal interactions and monitor the emissions at laboratory scale and Alcoa will verify the findings on commercial scale. The goal is to obtain a fundamental understanding, based on first principles, of the mechanisms for the pollutant formation that occurs when the salts are used in furnaces. This mechanistic information will be used to control process parameters so that emissions are consistently below the required levels. The information obtained in these experiments will be use for developing mathematical models that will help in optimizing the process.

Keywords: Salt Fluxing, Emissions, Primary Aluminum

99. **INERT METAL ANODES FOR PRIMARY ALUMINUM PRODUCTION**
$100,000
DOE Contact: Tom Robinson (202) 586-0139

Project partners will investigate inert anode systems to identify suitable candidate inert anode materials, test these materials in alumina electrolysis cells, and conduct post-test analyses of the anode materials, bath, produced metal, and cell hardware. Partners will focus on metal alloys as candidate materials, particularly alloys that form thin, self-limiting, self-healing alumina filMs. Selection and identification of suitable alloys will occur by measurement of their aluminum diffusion rates, film thickness, film dissolution rates, and thermodynamic properties. Most past and present investigations of inert anodes have focused on using ceramics and ceramic/metal materials. Metal anodes offer significant advantages including improved electrical conductivity, fracture toughness, thermal shock resistance, elimination of non-uniform current, and ease of fabrication into complex shapes for use in advanced cell designs. However, other than a few expensive noble metals, metals corrode in aluminum production cells. The project partners will develop a new inert hollow metal anode with a dissolving alumina surface film that is continuously replenished by aluminum additions to the interior of the anode. The role of the surface film is to protect the metal from corroding. In this project, metal alloys that form thin, self-limiting, self-healing alumina films will be evaluated for this new design.

Keywords: Inert Anodes, Alumina Electrolysis Cells, Ceramics, Fracture Toughness

100. **IMPROVED ENERGY EFFICIENCY IN ALUMINUM MELTING**
$190,000
DOE Contact: Tom Robinson (202) 586-0139

Reverberatory furnaces are the principal means used for melting aluminum. Project partners will investigate three dimensional models, improved sensor and control systems, and improved insulation and refractory materials, to optimize the melting efficiency of reverberatory furnaces (ERF) used for melting aluminum. An experimental ERF will be designed and built to conduct trials on combinations of oxy-fuel, staged combustion, new control systems, and new refractory materials and insulation. The most effective technology improvements will be demonstrated in cooperation with industry partners.

Keywords: Reverberatory Furnaces, Sensor and Control, Aluminum Melting

101. **EVALUATION AND CHARACTERIZATION OF IN-LINE ANNEALED CONTINUOUS CAST ALUMINUM SHEET**
$74,000
DOE Contact: Tom Robinson (202) 586-0139

For more than fifty years, the majority of aluminum strip, sheet and plate products have been produced by combinations of hot and cold rolling and annealing of large ingots. In contrast, aluminum sheet made by continuous casting provides an energy savings of at least 25 percent and an economic savings of more than 14 percent over sheet products made from an ingot. Formability is among the most important characteristics of aluminum sheet. Tensile and yield strength, ductility, and rates of work hardening control the complexity of the shapes that can be formed out of a sheet. Careful control of the final microstructure, texture, and strength throughout the sheet is required to give it good forming properties. Continuous cast aluminum sheet is directly cast, hot rolled and coiled. The sheet is not homogenized or held at a high temperature. This eliminates or decreases chemical segregation within the sheet before or during hot rolling. This structure characteristic is very important for aluminum alloys in subsequent processing. These alloys must have a uniform microstructure throughout the sheet in order to achieve the desired formability properties. The introduction of in-line heating/annealing prior to coiling could ensure optimum sheet formability. This project will develop in-line heating/annealing protocols for continuously cast aluminum sheet prior to coiling. The focus is on utilizing a process optimization model and increasing the understanding of the evolution of microstructure and microtexture in continuously cast sheet during in-line anneal. The implementation of this work will result in the production of continuous cast alloy sheet with improved formability at high levels of productivity, consistency and quality.

Keywords: Casting, Microstructure, Alloys, Formability

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

102. **SPRAY ROLLING ALUMINUM STRIP**
$150,436
DOE Contact: Tom Robinson (202) 586-0139
INEEL Contact: Kevin McHugh (208) 525-5713

Alcoa Incorporated, Century Aluminum, Colorado School of Mines, Idaho National Engineering and Environmental Laboratory, Inductotherm, Metals Technology, and University of California are project partners for the development of a new process that combines benefits of twin-roll casting and spray forming. Aluminum=s competitive edge arises from the ease with which shapes can be extruded. Nearly all aluminum strip is manufactured commercially by conventional ingot metallurgical (I/M) processing, also known as continuous casting. This method accounts for about 70 percent of domestic production. However, it is energy and capital equipment intensive. Spray forming is a competitive low-cost alternative to ingot metallurgy for manufacturing ferrous and non-ferrous alloy shapes. It produces materials with a reduced number of processing steps, while maintaining materials properties, with the possibility of near-net-shape manufacturing. However, there are several hurdles to large-scale commercial adoption of spray forming: 1) ensuring strip is consistently flat, 2) eliminating porosity, particularly at the deposit/substrate interface, and 3) improving material yield. Researchers are investigating a spray rolling approach to overcome these hurdles. It should represent a processing improvement over conventional spray forming for strip production. Spray rolling is an innovative manufacturing technique to produce aluminum net-shape products. It requires less energy and generates less scrap than conventional processes and, consequently, enables the development of materials with lower environmental impacts in both processing and final products. It combines benefits of twin-roll casting and conventional spray forming.

Keywords: Aluminum, Spray Forming, Aluminum Strip and Sheet

103. **MODELING OPTIMIZATION OF DIRECT CHILL CASTING**
$253,773
DOE Contact: Tom Robinson (202) 586-0139

The direct chill (DC) casting process is used for 68 percent of the aluminum ingots produced in the U.S. Ingot scrap from stress cracks and butt deformation account for a 5 percent loss in production. The basic process of DC casting is straightforward. However, the interaction of process variables is too complex to analyze by intuition or practical experience. The industry is moving toward larger ingot cross-sections, higher casting speeds, and an increasing array of mold technologies to increase overall productivity. Control of scrap levels is important in terms of both energy usage and cost savings. Predictive modeling and increasing the general knowledge of the interaction effects should lower production losses to 2 percent. This reduction in scrap could result nationally in an estimated annual energy savings of over six trillion Btu and cost savings of over $550 million by 2020. The DC casting model project focuses on developing a detailed model of heat conditions, microstructure evolution, solidification, strain/stress development, and crack formation during DC casting of aluminum. This model will provide insights into the mechanisms of crack formation, butt deformation, and aid in optimizing DC process parameters and ingot geometry. Project partners include Secat Inc., assisted by Alcan Aluminum Corp., ARCO Aluminum Inc., Logan Aluminum Inc., McCook Metals, LCC, Wagstaff Inc., Albany Research Co., Argonne National Laboratory, Oak Ridge National Laboratory, and University of Kentucky.

Keywords: Aluminum Ingot, Direct Chill Casting, Aluminum Scrap

104. **DEGASSING OF ALUMINUM ALLOYS USING ULTRASONIC VIBRATIONS**
$40,000
DOE Contact: Tom Robinson (202) 586-0139

The goal of this research is to understand fundamentally the effect of ultrasonic energy on the degassing of liquid metals and the development of practical approaches for the ultrasonic degassing of alloys. The result of ultrasonic use will be a degassing process in which less argon is needed and less aluminum is exposed to the furnace gases. This saves energy by reducing aluminum oxidation and the energy needed for argon production. This research will evaluate core principles and establish quantitative bases for the ultrasonic degassing of aluminum alloy melts, and demonstrate the application of ultrasonic processing during ingot casting and foundry shape casting. Important issues to be studied and solved include the coupling of the ultrasonic transducer to the melt, the effective transmission and distribution of ultrasonic vibrations in the melt, ultrasonic vibration intensity and frequency, and protection of the melt surface. The research will develop laboratory scale equipment for ultrasonic degassing, study the effect of process parameters, and identify the range of applicable process parameters for commercial implementation of the technology.

Keywords: Ultrasonic, Degassing, Casting

105. **EFFECT OF CASTING CONDITIONS AND COMPOSITION ON MICROSTRUCTURAL GRADIENTS IN ROLL CAST ALUMINUM ALLOYS**
$66,906
DOE Contact: Tom Robinson (202) 586-0139

Continuous roll casting of low alloy or unalloyed aluminum has been well established for several decades and has demonstrated energy savings of more than 25 percent relative to ingot rolling. There is great interest in extending this technology to the higher alloy series such as 5xxx and 6xxx to take advantage of the benefits of this process in high alloy products. This research is a comprehensive investigation of the effect of roll casting process conditions on the microstructure properties of relatively highly alloyed aluminum. The studies will determine the relationships between roll casting process parameters and the resulting microstructure, annealing response, and properties. In particular, the microstructural analysis will investigate the nature of the microstructural gradients that occur in these materials and the influence of these structures on recrystallization response, crystallographic texture, and formation of cracks during forming. The combined effects of alloying level and casting parameters on the resultant materials will be modeled.

Keywords: Microstructural, Alloys, Casting, Annealing

106. **ENERGY EFFICIENT ISOTHERMAL MELTING OF ALUMINUM**
$400,000
DOE Contact: Tom Robinson (202) 586-0139

The isothermal melting process (ITM) process saves half the energy and emissions associated with conventional melting. New materials and construction techniques for immersion heaters make ITM practical for large scale aluminum operations. Project partners will demonstrate ITM on a technically and commercially viable scale. Tasks include optimization of an immersion heater with composite refractory coating, design, construction and demonstration of a heating and charging chamber, and system integration and performance assessment at commercial scale. ITM will be implemented and demonstrated at a commercial aluminum casting facility.

Keywords: Isothermal Melting Process, Immersion Heater, Refractory

107. **COOLANT CHARACTERISTICS AND CONTROL IN DIRECT CHILL CASTINGS OF ALUMINUM**
$40,036
DOE Contact: Tom Robinson (202) 586-0139

Direct Chill (DC) casting is a critical process in the production of aluminum ingots. It is a casting process in which water-cooled molds initiate the first part of solidification. Thereafter, water sprays impinge on the shell of solid aluminum enclosing the liquid core. To obtain higher productivity and better quality products, it is important to precisely control the cooling rate in DC casting. Current methods of controlling the ingot cooling rate are empirical. A theoretical model based on system parameters and coolant characteristics has not been established. The cooling rate has a strong influence on the temperature, strain, and stress field in the cast product. A higher cooling rate can lead to higher thermal stresses and strains causing hot tearing and ingot cracking. This project focuses on understanding the fundamentals of coolant behavior and developing strategies to control the cooling rate of DC casting of aluminum ingots. Project partners will conduct a fundamental study to identify various parameters affecting critical heat flux and boiling transition and evaluate the effects of various additives (impurity particulates, sodium and calcium salts, carbonates, bicarbonates, surfactants, etc.). Partners will also study the effect of water quality on the ingot-cracking tendency. The research results are expected to guide cooling strategies, which can then control metallurgical characteristics and mechanical properties. This will result in better ingot yield from existing DC casting practices.

Keywords: Direct Chill Casting, Coolant Behavior

108. **CONTINUOUS SEVERE PLASTIC DEFORMATION PROCESSING OF ALUMINUM ALLOYS**
$384,000
DOE Contact: Tom Robinson (202) 586-0139

Ultrafine grained material allows the design and manufacture of aluminum components that use less metal and require fewer manufacturing steps. This provides energy and manufacturing cost savings. Several techniques for producing ultrafine grained materials are currently being investigated. These techniques are limited in their ability to produce the size and quantities of material needed for commercial use. One technique to produce ultrafine grained materials is the Equal Channel Angular Extrusion (ECAE) process. This technique is a multi-step batch process that produces small cross-section, short-length stock, which severely limits its commercialization. The Continuous Severe Plastic Deformation (CSPD) process will overcome the limitations of ECAE by producing large cross-section, continuous length stock. Project partners will develop the CSPD process for the production of continuous long lengths of bulk ultrafine grained aluminum alloys. Partners will demonstrate its feasibility in the laboratory and also demonstrate the advantages and use of the ultrafine grained material under industrial conditions. Using the CSPD process in place of conventional processes, and during secondary and finishing operations, will provide significant energy and cost benefits.

Keywords: Plastic Deformation, Ultrafine Grained Material

109. **DEVELOPMENT OF A ROLLING PROCESS DESIGN TOOL FOR USE IN IMPROVING HOT ROLL SLAB YIELD**
$200,000
DOE Contact: Tom Robinson (202) 586-0139

Multiple passes in a reversing rolling mill of a hot slab are used to produce semi finished aluminum plate. However, the large deformations encountered while rolling may lead to failure modes that result in loss of part or even the entire slab. The formation of defects within the plate, such as edge cracking, delamination, alligatoring (center splitting near the front and rear), and the formation of undesirable rolled end shapes, all lead to product losses. Critical equipment downtime is also associated with several failure modes. Typically, rolling plant yield from ingot to final production is about 50 percent. Rejected material is recycled and melted to form new ingots. Improving yield would lower the overall energy used in processing aluminum. The project goal is to develop a numerical modeling capability to optimize the hot rolling process used to produce aluminum plate. This tool will be used in the forming process so that loss of product will be minimized. Product lost in the rolling process requires the energy-intensive steps of remelting and reforming into an ingot. The modeling capability developed by project partners will be used to produce plate more efficiently and with better properties.

Keywords: Plastic Deformation, Ultrafine Grained Material

GLASS SUBPROGRAM

Energy expenditures account for nearly 15 percent of the production costs of glass products. The Glass Industry of the Future program works closely with the U.S. glass industry and other stakeholders to maintain a well-balanced portfolio of projects and services aimed at improving the performance of glass manufacturing facilities. Collaborative teams from industry, national laboratories, suppliers, universities, and other organizations share the risk and cost of R&D projects that are awarded from a competitive solicitation process. The DOE program manager is Elliott Levine (202) 586-1476.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

110. **DEVELOPMENT OF MODELS AND ON-LINE DIAGNOSTIC MONITORS OF THE HIGH-TEMPERATURE CORROSION OF REFRACTORIES IN OXY-FUEL GLASS FURNACES**
$200,000
DOE Contact: Elliott Levine (202) 586-1476
SNL Contact: Mark Allendorf (925) 294-2895

This research is directed toward understanding the mechanism(s) of enhanced refractory corrosion in oxy-fuel glass furnaces and the development of models to predict corrosion rates, identify operating regimes that minimize corrosion, and define the attributes of improved refractories. Activities in FY03 centered on conversion of analytical models to a software module for incorporation in a glass furnace code and field testing a monitor for gas-phase alkali detection.

Keywords: Refractories, Glass, Furnace, Oxy-Fuel, High Temperature, Properties, Corrosion, Monitor, Model

METAL CASTING SUBPROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

111. **CREEP RESISTANT ZINC ALLOY DEVELOPMENT**
$132,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
International Lead Zinc Research Organization Contact: Frank Goodwin (919) 361-4647

The objective of this project is to develop a hot chamber castable zinc die casting alloys that is capable of satisfactory service at 1400°C and preferably at moderately elevated temperatures 160°C. The target strength at this temperature is 4,500 psi during an exposure time of 1,000 hours. The project will be accomplished by enhancing a previously existing computer model relating zinc alloy composition to creep strength, followed by preparation of selected zinc die casting metal alloys and pressure die casting of these alloys. Mechanical testing will be carried out. An optimization task will then be conducted and these alloys will then be characterized in a manner similar to the first group of alloys. This task will be followed by technology transfer to die casters and their customers, concerning properties and processing of these enhanced alloys.

Keywords: Zinc Alloys, Zinc Die Casting, Creep Resistant

112. **DEVELOPMENT OF SURFACE ENGINEERED COATINGS FOR DIE CASTING DIES**
$244,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Colorado School of Mines Contact: John Moore (303) 273-3770

The objective of this research project is to develop a coating system that minimizes premature die failure (heat checking, erosive, and corrosive heat), and extend die life. No single (monolithic) coating is likely to provide the optimum system for any specific die casting application that will require its own specially designed "coating system". An optimized coating system will require a multi-layer "architecture" within which each layer provides a specific function, e.g. adhesion to the substrate, accommodation of thermal and residual stresses, wear and corrosion/oxidation resistance and non-wettability with the molten metal. The initial research project will concentrate on developing a coating system for dies used in die casting aluminum alloys. The measured outcomes from this research program will quantify comparisons of current aluminum die casting practice with the measured results using the newly developed coating systeMs. A comparison of cost/performance will also be determined for the new coating systems using current cost data as the base line.

Keywords: Surface Coatings, Multi-Layered-Surface Coatings, Die Casting, Die Casting Dies

113. **INTEGRATION OF RSP TOOLING WITH RAPID PROTOTYPING FOR DIE-CASTING APPLICATION**
$97,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Colorado State University Contact: James Folkstead (970) 491-7823

The objective of the project is to utilize a rapid-tooling technology that will reduce the lead time for prototype and production die-casting tooling starting from a CAD drawing. Currently, there is no commercially available rapid tooling technology that satisfies the needs of the die casting industry. Compared to rapid tooling technologies for plastic injection molding and other plastic forming methods, rapid tooling options for die casting are very limited.

Keywords: Metalcasting, Die Casting, Rapid Tooling

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

114. **CLEAN CAST STEEL: 1) MACHINABILITY OF CAST STEEL; 2) ACCELERATED TRANSFER OF CLEAN STEEL TECHNOLOGY**
$98,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates (205) 975-8011

This project is an extension to the Clean Cast Steel project, with the goal to improve casting product quality by removing or minimizing oxide defects and allowing the production of higher integrity castings for high speed machining lines. There are two objectives in this project, with the first one to identify the metallurgical factors influencing machinability of steel to gain an engineering understanding of the mechanism. A series of tests of commercial parts from participating foundries will be performed to evaluate the machinability. Factors to be examined include furnace practice, deoxidation practice, calcium wire injection, and heat treatment. The second objective is to provide the steel foundry industry with the technical resources needed to implement clean cast steel technology.

Keywords: Metalcasting, Steel Casting, Machinability

115. **PREVENTION OF POROSITY IN IRON CASTINGS**
$25,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Climax Research Services Contact: James Lakin
(248) 960-4900

The objective of this research project is to understand porosity formation in castings, to generate fundamental materials data relevant to porosity formation, and to develop a method by which metalcasters can predict the porosity problem and make the necessary adjustments to prevent it. This will be accomplished by developing an understanding of the mechanisms for pore formation in castings, and developing a model for the use of the metal casting industry. This model will take into account all the factors affecting porosity formation. This model will help iron foundries to predict the conditions that are conducive to porosity formation in castings, and to take measures to prevent porosity.

Keywords: Metalcasting, Cast Iron, Porosity

116. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$180,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact:
Charles Bates (205) 975-8011

The objective of this project is to advance the state of the art in Lost Foam Casting technology. It is being carried out at the Lost Foam Technology Center at the University of Alabama at Birmingham. The project provides a means for designers, manufacturers, and purchasers/users of cast metal parts to harvest the benefits of the lost foam process, and furnishes project participants the best available technology. The current research focus is on the general technical areas of casting dimensional precision and freedom from casting defects in aluminum and cast iron. Tasks include foam pyrolysis defects, coating technology, pattern materials and production, computational modeling, casting distortion, and technology transfer.

Keywords: Metalcasting, Lost Foam Casting

117. **METALLIC REINFORCEMENT OF DIRECT SQUEEZE DIE CAST ALUMINUM ALLOYS**
$100,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Case Western Reserve University Contact:
Jack Wallace (216) 368-4222

The objectives of the project are to: 1) develop commercially feasible methods of reinforcing aluminum die castings with strong, tough metal inserts, 2) select aluminum alloys for the matrix and customize the type of insert depending on the application, 3) optimize interfacial coatings to provide a strong metallurgical bond between the insert and aluminum alloy, and 4) evaluate the mechanical properties of the reinforced castings. Research includes fracture toughness and ballistic evaluation to be conducted at LANL.

Keywords: Metalcasting, Squeeze Casting, Aluminum, Reinforcement

118. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$120,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Tennessee Contact: Carl Lundin
(423) 974-5310

Duplex stainless steel castings are receiving greater attention since the use of wrought duplex components is on the increase. The duplex stainless steels are now often considered for severe service because of their unique properties with regard to corrosion resistance (especially pitting resistance), strength and toughness. Unfortunately, a standardized method does not currently exist for calibrating instruments for the direct assessment or measurement of the ferrite-austenite phase relationships. The objective of this project is to develop calibration standards that will be applicable to duplex stainless steel castings and which will cover the full spectrum of the traditional duplexes and the newly-introduced super duplex , which contains special alloy additions for enhanced properties.

Keywords: Metalcasting, Calibration, Duplex Stainless Steel

119. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$77,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Alabama - Birmingham Contact: Charles Bates (205) 975-8011

The primary focus of this project is to determine how the machinability of gray and ductile iron castings can be improved to support the development of thin walled gray and ductile iron castings for use in the ground transportation industry. Excessive microcarbides have been found in prior research to be a dominant factor degrading machinability of iron castings. One of the major emphases is to determine how the occurrence of microcarbides can be controlled by normal foundry processing changes.

Keywords: Metalcasting, Gray Iron, Cast Iron, Inclusions, Machinability

120. **IMPROVEMENTS IN SAND MOLD/CORE TECHNOLOGY: EFFECTS ON CASTING FINISH**
$106,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Ohio State University Contact: John Lannutti (614) 292-4903

The overall objective of the project is to develop a fundamental understanding of how sand structure controls the final casting finish of metal castings made using sand molds and cores. In this project, Ohio State University will undertake a study of the effects of mold/core uniformity by combining an advanced non-destructive x-ray analysis and an optical profiler. The project will generate a fundamental understanding of how metal surfaces form in contact with sand molds/cores. The effort will focus on chemically bonded sands.

Keywords: Metalcasting, Sand Mold, Casting Finish

121. **HEAT CHECKING AND WASHOUT OF SUPERALLOYS FOR DIE INSERTS**
$100,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Case Western Reserve University Contact: Jack Wallace (216) 368-4222

The project has three main objectives: 1) develop and evaluate nickle and cobalt-base superalloys for use as inserts in die casting of aluminum alloys, 2) design and run a full size "erosion test" for evaluating washout in die insert materials, and 3) study the mechanisms of thermal fatigue crack nucleation and propagation in superalloys and compare these to thermal fatigue cracking of steels.

Keywords: Metalcasting, Die Casting, Heat Checking, Inserts

STEEL SUBPROGRAM[8]

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

122. **CONTROLLED THERMO-MECHANICAL PROCESSING OF TUBES AND PIPES FOR ENHANCED MANUFACTURING AND PERFORMANCE**
$1,983,250
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
The Timken Company Contact: Robert Kolarik (330) 471-2378

This project has yielded a technology for generating targeted microstructures in the manufacture of tubes and pipes. The technology consists of an integrated control model that combines the results of metallurgical fundamental studies, models of the thermal and deformation processes, and product performance response relationships. One of the industrial research partners, The Timken Company, has installed the technology and expects annual savings of 70 million cubic feet of natural gas through reduced heat treating requirements. Timken is continuing to work collaboratively with Oak Ridge and Sandia National Laboratories and the Colorado School of Mines on additional models.

Keywords: Thermomechanical Processing, Modeling, Microstructure

[8]For every project within the American Iron and Steel Institute's (AISIs) Technology Roadmap Program (TRP), the funding shown is the total over the life of the project. Total DOE/ITP TRP funding in FY03 was $3,468,000.

123. **LIFE IMPROVEMENT OF POT HARDWARE IN CONTINUOUS HOT DIPPING PROCESSES**
$450,000
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
West Virginia University Contact: Keh-Minn Chang

The objectives of this project are to develop new bulk materials and surface treatment/coatings for life improvement of molten metal bath hardware and bearings in continuous hot-dip processes used for coating steel strip. The project goal is to result in extension of component life by an order of magnitude. Major progress has been made in developing materials to increase the life of molten zinc pot hardware on steel galvanizing lines by a factor of ten. Interest in this project is high because these high-speed hot dip lines often experience catastrophic component failures requiring shut down of the line. Steel industry hot dip operators are collaborating with researchers from West Virginia University, the Lead Zinc Research Organization Inc., and Oak Ridge National Laboratory.

Keywords: Pot Hardware, Hot Dip Processing, Lifetime

124. **PLANT TRIAL OF NON-CHROMIUM PASSIVATION SYSTEMS FOR ELECTROLYTIC TIN PLATE**
Total Project Budget under AISI/TRP: $248,508
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Weirton Steel Contact: John Sinsel (304) 797-2935
AISI Contact: Joe Vehec (412) 922-2772

The successful completion of the project “Development of a Chromium-Free Passivation Treatment of Electrolytic Tin Plate (ETP),” has resulted in the identification of three non-chromium passivation systems: 1) British Steel Tinplate Experimental System #2 (zirconium sulfate); 2) Betz Dearborn Permatreat 1001 (zirconium-based proprietary treatment); and 3) PPG Chemfil Nupal (total organic proprietary treatment). All three systems exhibited acceptable performance in various tests, but showed some susceptibility to sulfide staining. The goal of this follow-on project is to complete a plant trial comparing three previously developed non-chromium passivation treatments for electrolytic tin plate and to thoroughly evaluate these processes to determine their viability.

Keywords: Electrolytic Tin Plate, Passivation, Chromium-Free

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

125. **RESEARCH RELATED TO THE DEVELOPMENT OF THE AUTOMATED STEEL CLEANLINESS ANALYSIS TOOL (ASCAT)**
$300,000
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
RJ Lee Group Contact: Gary Casuccio (724) 387-1818

The goal of this project is to research inclusion characterization, develop an automated steel cleanliness analysis tool (ASCAT) that will allow steel producers to evaluate steel quality during production, and demonstrate the unit in up to two steel mills. The project has five major areas of investigation: 1) development of rapid, near real time, analysis tool capable of locating, sizing, and identifying critical defects; 2) development of a methodology for the extraction and preparation of samples from liquid steel for analysis of their inclusion distributions; 3) testing of a rugged ASCAT system to gather data in steel mills; 4) data analysis to develop and quantify benefits and determine performance characteristics for ASCAT; and 5) introduction of ASCAT as part of the steel production process in the steel mill environment.

Keywords: Steel, Automation, Cleanliness Analysis

126. **ENHANCED INCLUSION REMOVAL FROM STEEL IN THE TUNDISH**
Total Project Budget under AISI/TRP: $813,045
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
University of Alabama Contact: R.C. Bradt (205) 348-0663
AISI Contact: Joe Vehec (412) 922-2772

The goal of this project is to determine the potential for delivery of molten steel with significantly reduced inclusion content from the tundish to the continuous casting mold. The project focuses on three major areas of investigation: modifying a commercially available computation fluid dynamics code for the specific flow conditions of the project; modeling dispersed liquid metal/particle turbulent flow in corrugated channels; and preparing corrugated channels and evaluating them at laboratory scale and performing field tests in sponsoring steel companies' tundishes.

Keywords: Computational Fluid Dynamics, Modeling, Inclusion Removal

127. **REDUCING THE VARIABILITY OF HSLA SHEET STEELS**
Total Project Budget under AISI/TRP: $548,168
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
University of Pittsburgh Basic Metals Processing Research Institute Contact: Anthony DeArdo
AISI Contact: Joe Vehec (412) 922-2772

The goal of this project is to identify the relative influence of different hot mill processing steps on the yield strength variability of an HSLA steel and to recommend changes in chemistry that will reduce such variability. One source of the variability in the strength of HSLA steel is the fluctuation of processing in the hot strip mill. Working with a 70-ksi HSLA steel, the variations in the evolution of microstructure during laboratory hot-rolling can be monitored as different levels of reheating, roughing, finishing, and coiling temperatures are used. Measurement of the mechanical properties of the hot band and the subsequently cold-rolled and annealed strip allows identification of the processing steps responsible for the major portion of the property variability. This variability can then be linked to the observed changes in microstructure during processing. From prior knowledge of the interdependence of microstructure, processing variables, and chemistry, recommended ways to adjust the steel chemistry have emerged.

Keywords: High-Strength Steels, Variability

128. **CONSTITUTIVE BEHAVIOR OF HIGH STRENGTH MULTIPHASE SHEET STEELS UNDER HIGH STRAIN RATE DEFORMATION**
Total Project Budget under AISI/TRP: $1,023,060
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Colorado School of Mines Contact: Dr. David K. Matlock , dmatlock@mines.edu
AISI Contact: Joe Vehec (412) 922-2772

The focus of this research program is to systematically assess the strain rate dependence of strengthening mechanisms (e.g. ferrite grain size, cold work, solid solution strengthening, low-temperature aging, martensite properties and volume fraction, and amount and stability of retained austenite) in new advanced high-strength sheet steels. Data are being obtained on specially designed and produced Dual-Phase and TRIP steels and compared to properties of current automotive sheet steels (e.g.IF, HSLA, AKDQ, etc.). Tensile data have been obtained on a variety of sheet steels including IF, HSLA, TRIP, and Dual-Phase. The results of this research are being incorporated into constitutive material behavior models used in the vehicle design/development process for forming and crash simulations.

Keywords: High-Strength Steels, Strain Rate Deformation, Constitutive Models

129. **CLEAN STEEL – ADVANCING THE STATE OF THE ART**
Total Project Budget under AISI/TRP: $421,612
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Carnegie Mellon University Contact: Alan W. Cramb (412) 268-5548
AISI Contact: Joe Vehec (412) 922-2772

The future of steelmaking and casting will be to continue to reduce the total oxide inclusion mass in liquid steels and to ensure that the remaining inclusion chemistry and size distribution is closely controlled. The purpose of this project is to determine the potential limiting factors in the production clean steels and to produce on the laboratory scale ultra clean steels beyond that currently available in bulk production. This project will lead to the development of processes or process strategies that will allow cleaner more consistent steels to be produced. Specifically, the goals are to determine the kinetic factors governing inclusion removal from liquid steels at a slag metal interface, to develop a methodology to enable steels of less than 1 ppm total oxygen to be produced with an average inclusion diameter of less than 5mm, and to determine the slag-metal interface conditions necessary for ultra clean steels.

Keywords: Steel, Inclusion Removal

130. **CHARACTERIZATION OF FORMABILITY OF ADVANCED HIGH STRENGTH STEELS**
Total Project Budget under AISI/TRP: $1,007,959
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Ispat Inland Research Laboratories Contact: Sriram Sadagopan (219) 399-5593
AISI Contact: Joe Vehec (412) 922-2772

This project has delivered comprehensive data on the formability of a new generation of high-strength steels, including dual phase and TRIP steels, and will make it possible to evaluate FEA formability methods for both breakage and distortion. The project consisted of a series of tests on controlled lots of steel to accurately measure their stretching and drawing characteristics, formability limits, stress/strain, and distortional properties. Project results characterized the formability of high-strength steels by using a series of simulative tests that provide data on comparative performance, by providing high quality data to evaluate FEA formability methods, for both breakage and distortion (springback, etc.), and by providing more sophisticated stress-strain data as a basis for understanding differences in behavior in the simulative tests and as input for FEA.

Keywords: High-Strength Steels, Formability

131. **DEVELOPMENT OF A STANDARD METHODOLOGY FOR QUANTITATIVE MEASUREMENT OF STEEL PHASE TRANSFORMATION KINETICS AND DILATION STRAINS USING DILATOMETRIC METHODS**
Total Project Budget under AISI/TRP: $1,152,348
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
National Center for Manufacturing Sciences Contact: Manish Mehta (734) 995-4938
AISI Contact: Joe Vehec (412) 922-2772

The purpose of this collaborative project is to develop a standard practice for obtaining and archiving quantitative steel transformation kinetic and thermal strain data. The initial thrust is focused on bar and rod product forms of steel. Parallel standard development paths are being pursued to cover two families of dilatometric equipment: 1) high-speed quenching and deformation dilatometers, and 2) Gleeble thermo-mechanical processing equipment. The standard practice methodologies will be developed for three distinct austenite transformation scenarios (transformation of the austenite under no applied elastic stress or plastic deformation, transformation while a static elastic stress is applied to the austenite, and transformation of the austenite while it is undergoing plastic deformation).

Keywords: Steel, Transformation, Dilatometer, Gleeble

132. **CHARACTERIZATION OF FATIGUE AND STRESS/STRAIN BEHAVIOR IN ADVANCED HIGH STRENGTH STEELS**
Total Project Budget under AISI/TRP: $385,221
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Ispat Inland Research Laboratories Contact: Benda Yan
AISI Contact: Joe Vehec (412) 922-2772

A two-year project to generate fatigue and high strain data for a new generation of high strength steels (HSS) was completed in December 2002. The project tested eleven steel grades, including Dual Phase (DP) steels, Transformation-Induced Plasticity (TRIP) steels, Bake Hardenable (BH) steels, and conventional High Strength Low Alloy (HSLA) steels. In addition to the fatigue data and high strain rate data generated for the steels studied in the project, analyses of the testing results revealed that Advanced High Strength Steels (AHSS) exhibit significantly higher fatigue strength and crash energy absorption capability than conventional HSS. TRIP steels exhibit exceptionally better fatigue strength than steels of similar tensile strength but different microstructure, for conditions with or without notches present.

Keywords: High-Strength Steels, Fatigue, Stress-Strain Behavior

133. **VALIDATION OF HOT STRIP MILL MODEL**
Total Project Budget under AISI/TRP: $2,594,476
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
INTEG Process Group Contact: Richard Shulkosky (724) 933-9350
AISI Contact: Joe Vehec (412) 922-2772

The objective of the project is to take the hot strip mill model developed by the University of British Columbia under the AISI/DOE Advanced Process Control Program from 1993-1998 to test, upgrade and validate the core models used for predicting the temperature, forces, microstructure evolution and final mechanical properties of steel produced on a hot strip mill. At the conclusion of the original program, INTEG process group, inc. was selected as the commercialization partner for the model. An enhancement group consisting of several of the original sponsoring steel companies was formed in 2000 to further develop, test and validate the models. The scope of the current effort work includes validating and/or replacing various sub-models, adding practical application functions, updating the users interface to facilitate the ease of use of the model and to provide adequate documentation.

Keywords: Steel, Hot Strip Mill, Modeling

134. **INCLUSION OPTIMIZATION FOR NEW GENERATION STEEL PRODUCTS**
Total Project Budget under AISI/TRP: $448,210
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Carnegie Mellon University Contact: Alan W. Cramb (412) 268-5548
AISI Contact: Joe Vehec (412) 922-2772

The objective of this project, which is being sponsored by the Department of Materials Science and Engineering at Carnegie Mellon University and several steel companies, is to determine what conditions best lead to the formation of beneficial inclusions in liquid steels. Additionally, researchers are seeking to determine the processing conditions during casting that will allow these inclusions to become nucleants for solidification and subsequent solid state phase transformations. This study will result in a new understanding of the role of inclusions in steel production and will be the foundation of the inclusion engineered steels that are required for current and future casters.

Keywords: Steel, Inclusion Optimization

135. **DEVELOPMENT OF APPROPRIATE SPOT WELDING PRACTICE FOR ADVANCED HIGH STRENGTH STEELS**
Total Project Budget under AISI/TRP: $235,090
DOE Contact: Simon Friedrich (202) 586-6759
Edison Welding Institute Contact: Warren Peterson (614) 688-5261
AISI Contact: Joe Vehec (412) 922-2772

Although the mechanical characteristics of Advanced High Strength Steels (AHSSs) are extremely beneficial for achieving automotive light-weighting goals, improving body strength, and safety, they come with their own set of complications. Resistance spot welding is the most widely used joining method for auto body construction. A phenomenon known as hold-time sensitivity (HTS) has long been known to be a concern when spot welding steel with high C and Mn levels, such as those found in the AHSSs. Studies at Edison Welding Institute (EWI) have developed some understanding of the relationship between steel composition, process variables, and HTS. For higher carbon steels, HTS was largely related to weld metal hardness. Relatively large changes in weld hardness could result from even small variations in carbon content. Additionally, lighter steel gauges increase weld metal hardness compared to thicker gauges.

Keywords: High-Strength Steels, Spot Welding

MATERIALS PREPARATION, SYNTHESIS DEPOSITION, GROWTH OR FORMING

136. **IRONMAKING CHALLENGE – THE MESABI NUGGET RESEARCH PROJECT**
$3,596,540
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Mesabi Nugget, LLC Contact: Larry Lehtinen (218) 226-6206

The Mesabi Nugget Project is a large-scale program to demonstrate the ITmk3 Process developed by Kobe Steel, Ltd. The ITmk3 Process is a new ironmaking technology that uses a rotary hearth furnace to turn iron ore fines and pulverized coal into iron nuggets of similar quality as blast furnace pig iron. The direct use of coal to make iron is an alternative to the current prevailing ironmaking practice that uses coke made from coal. The high-quality, low-cost nuggets can be fed into either a basic oxygen furnace or an electric arc furnace. A pilot demonstration plant in Silver Bay, Minnesota is currently on its third campaign; in previous campaigns, the plant operated continuously for at least thirty days, producing over 1,000 tons of iron. The purity (metallic iron content) of the test nuggets has exceeded 95 percent. The purpose of the project is to assess process conditions for producing iron nuggets that can be fed into a commercial steelmaking furnace. Participants include Mesabi Nugget LLC, Kobe Steel USA, the State of Minnesota, Cleveland Cliffs, and Steel Dynamics.

Keywords: Ironmaking, Rotary Hearth, Mesabi Nugget Project

137. **DEVELOPMENT OF STEEL FOAM MATERIALS AND STRUCTURES**
Total Project Budget under AISI/TRP: $822,000
DOE Contacts: Simon Friedrich (202) 586-6759 and Debo Aichbhaumik (303) 275-4763
Fraunhofer USA Contact: Ken Kremer (302) 369-6761
AISI Contact: Joe Vehec (412) 922-2772

The objective of this project is to develop steel foam materials and structures based on Fraunhofer's patented powder metallurgy-based process. Thus far, progress has been made in reducing the carbon content from 2.5 percent to below 1.0 percent while maintaining densities at 50 percent and lower. This has also enabled the development of more useful microstructures that will yield better properties. Improvements in forming and processing have produced a more spherical pore shape and uniform pore size distribution in the foamed steel that will perform in a more predictable and consistent manner. Simple geometry components have been produced. A mechanical and physical properties database is being built that will allow design and application of lightweight steel with a controlled pore structure.

Keywords: Steel, Foam, Powder Metallurgy

MATERIALS SUBPROGRAM

New or improved materials can save significant energy and improve productivity by enabling systems to operate at higher temperatures, last longer, and reduce capital costs. The Industrial Materials for the Future (IMF) program is a crosscutting program with emphasis on meeting the industrial needs of the Industries of the Future (IOFs) effort and of crosscutting industries including the forging, heat treating, process heating, powder metallurgy, welding, and carbon products industries. Efforts in FY 2003 were focused on the research, design, development, and testing of new and improved materials, as well as more profitable uses of existing materials, for the IOFs. The projects are grouped in the following categories 1) Degradation Resistant Materials 2) Databases and Modeling 3) Materials for Separations, and 4) Materials for Engineering Components and project descriptions are included below. The DOE program manager is Sara Dillich (202) 586-7925.

DEGRADATION RESISTANT MATERIALS

COATINGS AND SURFACE MODIFICATIONS

138. **ADVANCED COMPOSITE COATINGS FOR INDUSTRIES OF THE FUTURE**
$660,000
DOE Contact: Sara Dillich (202) 586-7925
PNNL Contact: Charles Henager, Jr., (509) 376-1442

The goal of the project is to develop low-cost, ceramic coatings for prevention of high-temperature corrosion of metals and ceramics in industries such as chemical processing and industrial power generation. These coatings are targeted at providing high-temperature (700–1000˚C) protection from corrosion due to oxidation, carburization, coking, and metal dusting. Coatings are being fabricated by pyrolysis of preceramic precursors and in situ displacement reactions. Both routes require a thorough understanding of the materials development during coating fabrication and the properties of the material that control the coating behavior. In addition to pursuing these two coating techniques, composite coatings are being developed as a means to further improve coating performance. The composite coatings consist of preceramic polymer-derived or in situ displacement reaction material combined with additional constituents that can improve corrosion resistance, mechanical properties, and thermal properties. Tasks include development of corrosion resistant compositions, coating adhesion, and characterization and optimization for service environments.

Keywords: Coatings, Mechanical Properties, Ceramics, Pyrolysis, Corrosion Resistance, Thermal Properties

139. **DEVELOPMENT OF ULTRANANOCRYSTALLINE DIAMOND (UNCD) COATINGS FOR SIC MULTIPURPOSE MECHANICAL PUMP SEALS**
$500,000
DOE Contact: Sara Dillich (202) 586-7925
ANL Contact: John Hryn (630) 252-5894

The objectives of this project are to (a) understand the fundamental processes involved in the growth of UNCD coatings (b) develop a technological base for UNCD applications, and (c) demonstrate the applicability of UNCD coatings in industrial applications, such as multipurpose mechanical pump seals. Until recently, control of diamond microstructure was limited to affecting the crystal orientation (texturing) but not, in a significant way, the crystallite size. A major advance was achieved at Argonne National Laboratory recently, when it was discovered that diamond film microstructure could be controlled so that crystallite size spans the range from the micron to the nanometer size, a factor of a million in volume. In order to apply this technology to commercial applications, such as pump seals, work is being performed on plasma physics and chemistry, diamond seeding processes on substrate surfaces, and film growth processes to produce UNCD layers on large area substrates with uniform thickness and microstructure.

Keywords: Coatings, Chemical Vapor Deposition (CVD), Ultrananocrystalline Diamond, Plasma Processing

140. **HIGH DENSITY INFRARED (HDI) TRANSIENT LIQUID COATINGS (TLC) FOR IMPROVED WEAR AND CORROSION RESISTANCE**
$300,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The project's aims are to 1) develop, evaluate, and understand how high density infrared heating technology can improve infiltrated carbide wear coating systems and 2) better understand the densification and metallurgical bonding of thermal spray coatings. HDI/TLC systems that are capable of fusing carbide coatings for industrial applications are being developed. Engineering development is focused on the process and equipment technology necessary to implement industrial HDI/TLC systems that can fuse coatings on parts such as agricultural blades, rolls for metallurgical processing, and components for paper and polymer processing. Fundamental research is aimed at understanding the effect of HDI/TLC processing on the coating materials and the subsequent coating properties. The expected outcome of this work is the development of the necessary materials and process knowledge to specify the coating precursor and enable the control of the HDI/TLC process.

Keywords: High Density Infrared Heating Technology, Transient Liquid Coatings, Thermal Spray Coatings, Bonding, Corrosion Resistance, Wear

141. **HIGH ENERGY DENSITY COATING OF HIGH TEMPERATURE ADVANCED MATERIALS FOR ENERGY EFFICIENT PERFORMANCE**
$125,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069
University of Tennessee Contact: Narendra Dahotre (865) 974-3609

The goal of the project is to develop a reliable, efficient, and economic method of coating metal using high-energy-density UV laser and IR lamp techniques. Intermetallic FeAl coatings have been processed using laser and IR based techniques and the microstructure characterized. Composite coatings, comprised of hard ceramic particles in a steel matrix, have also been deposited. The phases have been identified; the microhardness has been measured, and wear tests performed. Additional coating trials using different process energy levels will be performed and the resultant coatings characterized. The process and coating-substrate material systems will be optimized to suit specific industrial applications.

Keywords: Advanced Materials, Wear, Corrosion, UV Laser Processing, IR Processing, Composite Coatings

MATERIALS DEVELOPMENT AND PROCESSES

142. **ADVANCED NANOPOROUS COMPOSITE MATERIALS FOR INDUSTRIAL HEAT APPLICATIONS**
$300,000
DOE Contact: Sara Dillich (202) 586-7925
Lawrence Berkeley National Laboratory Contact:
Arlon Hunt (510) 486-5370

The goal of the project is to develop new insulating mesoporous composite materials for process-heating applications. The major objective of this project involves developing aerogel composite materials that retain the advantageous properties of standard aerogels while increasing their mechanical and chemical compatibility properties to the levels necessary to meet the needs of various IOF industries. The approach for creating composite materials with tailored thermal and mechanical properties is based on sol-gel technology, which will be used to create refractory multicomponents from a porous monolithic gel, followed by supercritical solvent extraction. Post-processing techniques, including chemical vapor infiltration and advanced packaging processes, will also be developed. The packaging processes include the incorporation of fibrous or particulate materials as mechanical enhancements and infrared opacifants, exterior dense oxide coatings, and shaping/forming processes. Aerogels similar in composition to the oxide ceramics used today for refractories will be prepared, and their thermal and mechanical properties will be evaluated. Various nanostructured materials have been evaluated for their suitability for use in insulation panels and refractory blocks and samples will be prepared for thermal conductivity measurements.

Keywords: Nanoporous, Advanced Composite Materials, Mesoporous, Process Heating, Aerogels, Sol-Gel, Refractories, Monolithic Gel, Chemical Vapor Infiltration, Fibrous Materials, Infrared Opacifants, Coatings, Ceramics, Mechanical Properties

143. **CROSSCUTTING INDUSTRIAL APPLICATIONS OF A NEW CLASS OF ULTRA-HARD BORIDES**
$2,866,403
DOE Contact: Sara Dillich (202) 586-7925
Ames Laboratory, Iowa State University Contact:
Bruce Cook (515) 294-9673

The goal of this project is to develop a new class of ultra-hard materials, based on the complex boride $AlMgB_{14}$, into high-performance, cost-effective solutions for a wide range of key industrial focus areas, including metalcasting, forest products, mining, and agriculture. Some of the challenges to be addressed in the development of the new $AlMgB_{14}$ technology will be to understand and control the formation of deleterious oxide phases during processing, to identify appropriate large-scale mechanical alloying techniques best suited for processing nanometric boride, and to characterize properties such as its low ductility and impact resistance (fracture toughness). Mechanical alloying experiments followed by hot pressing and materials analysis have been performed to determine the processing conditions necessary to create the desired microstructure. $AlMgB_{14}$ coatings have been prepared by a pulsed laser deposition process and will be characterized.

Keywords: Borides, Abrasive Wear, Ductility, Fracture Toughness, Mechanical Alloying, Pulsed Laser Deposition, Coatings

144. **DEVELOPMENT OF A NEW CLASS OF Fe-3Cr-W (V) FERRITIC STEELS FOR INDUSTRIAL PROCESS APPLICATIONS**
$375,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The objective of this project is to develop a new class of Fe-3Cr-W(V) ferritic steels for chemical process applications, industrial heat recovery boilers, and hoods for steel making furnaces. Target characteristics for the new class of Fe-3Cr-W(V) steels include 1) 50% higher tensile strength at temperatures up to 650˚C than current alloys 2) potential for not requiring any post weld heat treatment 3) equipment weight reduction of 25%, and 4) impact properties of approximately 100 ft-lb and -10˚F (-20˚C) for upper shelf energy and ductile to brittle transition temperature, without tempering treatment. The project objectives are being met through a range of concepts: 1) alloy composition optimization through the use of thermodynamic/ kinetic modeling 2) development of time-temperature-transformation curves for defining selective heat-treatment conditions 3) melting and processing laboratory and large-scale heats 4) welding and fabrication process development 5) physical and mechanical properties of base and weldments, and 6) testing of prototype components and preparation of data packages for ASTM and ASME Code approvals.

Keywords: Ferritic Steels, Tensile Strength, Alloys, Thermodynamic Modeling, Welding, Mechanical Properties

145. **DEVELOPMENT OF STRONGER AND MORE RELIABLE CAST AUSTENITIC STAINLESS STEELS (H-SERIES) BASED ON SCIENTIFIC DESIGN METHODOLOGY**
$175,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The goal of this project is to increase the high-temperature creep strength by 50 percent and the upper-use temperature by 30 to 60˚C for HP-modified and 100 to 200˚C for modified HK cast austenitic stainless steels. The R&D utilizes alloy design methods developed at Oak Ridge National Laboratory (ORNL), based on precise micro characterization and identification of critical microstructure/ properties relationships, and on combining them with the modern computational science-based tools that enable the prediction of phases, phase fractions, and phase compositions based on alloy compositions. The combined approach of micro characterization of phases and computational phase prediction will permit rapid improvement of a current class of alloy compositions with the long-term benefit of customizing alloys within grades for specific applications. Experimental alloys have been prepared based on the compositions determined by the thermodynamic and kinetic modeling and high temperature creep data is being collected.

Keywords: Stainless Steel, Modeling, Microstructure, Creep, Metallic Phases, Alloying

146. **EXPLORING ULTRAHIGH MAGNETIC FIELD PROCESSING OF MATERIALS FOR DEVELOPING CUSTOMIZED MICROSTRUCTURES AND ENHANCED PERFORMANCE**
$200,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The principal objective of this project is to evaluate magnetic processing as a viable and robust new technology for altering phase equilibria and phase transformation kinetics in a ferrous alloy with the goal of developing novel microstructures and properties unattainable through conventional thermomechanical processing approaches. The secondary objective is to develop the predictive capability to establish the influence of an applied magnetic field on ferrous alloys with the ability to extend this capability to more general ferromagnetic, paramagnetic, and diamagnetic materials. Ferrous alloys are being studied initially since this alloy family exhibits ferromagnetism over part of its temperature range of stability and therefore would demonstrate the maximum impact of this novel processing mechanism. Thermodynamic calculation capability will be developed to enable parametric studies to be performed to predict the magnitude of the influence of magnetic processing variables on the phase stability in paramagnetic and diamagnetic materials of relevance to the Industries of the Future.

Keywords: Ferromagnetism, Paramagnetism, Microstructures, Ferrous Alloys, Magnetic Field Processing, Phase Equilibria, Transformation Kinetics

147. **NOVEL SUPERHARD MATERIALS AND NANOSTRUCTURED DIAMOND COMPOSITES FOR MULTIPLE INDUSTRIAL APPLICATIONS**
$716,000
DOE Contact: Sara Dillich (202) 586-7925
Los Alamos National Laboratory Contact: Zhao Yusheng (505) 667-3886

The goal of this R&D project is to synthesize novel superhard B-C-N materials and to manufacture nanostructured diamond/SiC composites. The project covers a broad research scope of high-pressure, high-temperature synthesis, property characterization, and industrial implementation. The successful synthesis of the superhard B-C-N materials and nanostructured diamond/SiC composites will require a) advanced high-pressure techniques with the use of a unique Pt capsule to confine the volatile phases b) the effective use of suitable solvents and catalysts to promote synthesis reaction and crystallization, and c) the appropriate selection of the composition and particular preparation of starting materials. Studies are being conducted on the correlation between hardness, elastic moduli, crystal structure, thermal stability, chemical composition, and physical properties. Hybrid micron-/nano-diamond composites with nanostructure SiC matrix have enhanced fracture toughness values.

Keywords: Diamond Composites, Superhard Materials, Nanostructure, Solvents, Catalysts, Crystallization, High Pressure Techniques, SiC, Fracture Toughness, Grain Size

148. **ULTRASONIC PROCESSING OF MATERIALS**
$100,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The objectives of this project are to develop core principles and establish a quantitative basis for nucleation, growth, and fragmentation processes during alloy solidification in an acoustic field. Key areas of interest during ultrasonic processing are 1) grain refinement of alloys during solidification, and 2) degassing of alloy melts. The study is focused on aluminum alloys and specialty steels, and will analyze the application of ultrasonic processing during ingot and continuous casting, foundry shape casting, and vacuum arc remelting. Metal mold casting experiments have been performed under different ultrasonic conditions, such as casting temperature, vibrational amplitude and vibration duration time.

Keywords: Ultrasonic Processing, Alloys, Metals, Grain Refinement, Degassing, Casting, Steel

149. **FRACTURE TOUGHNESS AND STRENGTH IN A NEW CLASS OF BAINITIC CHROMIUM-TUNGSTEN STEELS**

$124,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The goal of this project is to understand the toughening and strengthening of the new Fe-3Cr-W (V) steels and weldment so as to optimize the microstructure through heat treatment and compositional design of the steels. The project focuses on high fracture toughness and strength for a new class of Fe-3Cr-W (V) steels through understanding of their toughening and strengthening mechanisMs. This class of steels has 1) 50% higher tensile strength at temperatures up to 550 to 600˚C than current alloys 2) high fracture resistance, and 3) potential for not requiring any postweld heat treatment (PWHT). However, this new class of Fe-3Cr-W(V) steels is not of sufficient maturity due to lack of understanding of the 1) microstructure-controlled strengthening and toughening, which can lead to further development of the steels, and 2) the fracture toughness relationship with microstructure in weldments before and after PWHT. Fe-3Cr-W(V) steel specimens are being prepared at ORNL by vacuum arc melting, solidification, hot rolling, austenitizing at 1050˚C, and normalization in argon. Some samples were tempered and their embrittlement behavior analyzed. The University of Pittsburgh is performing the microstructure characterization by the use of transmission electron microscopy (TEM) and energy-dispersive spectroscopy (EDS). They are measuring the tensile properties and characterizing the microstructure of prestrained specimens. The fracture toughness is being measure by performing J_{IC} tests and atomic force microscopy (AFM) is being used to analyze the area near the crack tip.

Keywords: Steel, Vacuum Arc Melting, Tensile Strength, Fracture Toughness, Heat Treating, Microstructure Characterization, Alloys

REFRACTORIES

150. **DEVELOPMENT OF COST EFFECTIVE CERAMIC AND REFRACTORY COMPONENTS FOR ALUMINUM MELTING AND CASTING**
$300,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The focus of this project is to develop and validate new classes of cost effective low-permeability ceramic and refractory components for handling molten aluminum in both smelting and casting environments. The primary goal is to develop materials and methods for sealing surface porosity in thermal shock- resistant ceramic refractories, which will also include the evaluation of monolithics used in the low-pressure casting of aluminum. The approach includes understanding the failure mode of refractory tubes in molten aluminum, characterizing the porosity in delivery tubes, evaluating monolithic tube materials, developing and optimizing the surface modification process to close the porosity, and choosing a refractory powder blend that minimizes the porosity. Several semicrystalline glazes have been prepared and are being analyzed. Dip, spray, and brush methods for applying the glazes have been investigated.

Keywords: Aluminum, Casting, Ceramic, Refractories, Glazes, Monolithics, Tubes, Porosity

151. **HIGH DENSITY INFRARED TREATMENT OF REFRACTORIES**
$200,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The goal of the project is to make a major advancement in improving the behavior of refractory materials used in industrial processes. The project is being performed as a series of tasks. The objectives of the tasks are 1) demonstrate the ability to reduce open surface porosity on commercially available refractories and evaluate the corrosion behavior 2) fabricate corrosion-resistant surface layers on refractories by either diffusion coating or selective sintering of secondary layers, and 3) produce refractories having high-emissivity surface coatings (in addition to low porosity and high corrosion resistance). Zirconia and spinel coatings were applied to aluminosilicate and MgO based refractory materials by a slurry technique and then subjected to high density infrared treatments to bond the coatings to the refractory. The corrosion resistant behavior will be studied.

Keywords: Infrared, Refractories, Porosity, Corrosion Resistance, Coatings, Sintering, Aluminosilicate, Magnesia

DATABASES AND MODELING

152. **THERMOCHEMICAL MODELS AND DATABASES FOR HIGH TEMPERATURE MATERIALS PROCESSING AND CORROSION**
$1,000,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069
Sandia National Laboratories Contact:
Mark Allendorf (925) 294-2895

The goal of the project is to greatly improve the availability, accuracy, and accessibility of thermochemical property data required to understand, simulate, and optimize industrial processes involving glass and refractory materials at high temperatures. The objective is to employ advanced computational techniques to develop a coherent database of thermochemical values and sets of models for gas and condensed-phase systems of importance to the processing of glass and to the industrial use of refractories. The product will be a web-based database/model information site that will provide the necessary input for commercial application.

Keywords: Glass, Refractory, Thermochemical, High Temperature, Advanced Computational Techniques, Corrosion, Materials Processing

153. **DEVELOPMENT OF COMBINATORIAL METHODS FOR ALLOY DESIGN AND OPTIMIZATION**
$200,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

This project aims to develop a comprehensive methodology for designing and optimizing metallic alloys by combinatorial principles. Combinatorial methods promise to significantly reduce the time, energy, and expense needed for alloy design, largely because conventional techniques for preparing alloys are unavoidably restrictive in the range of alloy compositions that can be examined. The basic concept is to develop a technique that can be used to fabricate an alloy specimen with a continuous distribution of binary and ternary alloy compositions across its surface–an "alloy library"–and then use spatially resolved probing techniques to characterize the structure, composition, and relevant properties of the library. As proof of principle, the methodology will be applied to the Fe-Ni-Cr ternary alloy system that constitutes the commercially important H-series and C-series heat- and corrosion-resistant casting alloys. Combinatorial methods will also be developed to assess the resistance of these materials to carburization and aqueous corrosion, properties important in their application. Some alloy libraries have been prepared by thin film deposition and annealing. Nanoindentation measurements will be performed.

Keywords: Combinatorial, Alloy Design, Carburization, Corrosion

154. **INVERSE PROCESS ANALYSIS FOR THE ACQUISITION OF THERMOPHYSICAL PROPERTY DATA**
$200,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The goal of this project is to improve the acquisition of data on thermophysical properties such as solid fraction and density during solidification, by developing realistic thermal models and concurrently using inverse-type computational analyses of the measurement process. New computational methodologies and measurement procedures will be developed to obtain accurate data on thermophysical properties. Methodologies include high-heat-flux differential scanning calorimetry (DSC) and dual-push-rod dilatometer analyses. By performing a computational analysis of the measurement process, the time lag and thermal resistances can be estimated and their effect can be taken into account in determining more accurate data on thermophysical properties. The tasks include 1) developing analytical models for DSC 2) developing analytical models for dilatometry 3) conducting DSC and dilatometry measurements 4) experimentally validate the proposed methodologies, and 5) evaluation of experimental and computational procedures.

Keywords: Dilatometry, Thermophysical Properties, Differential Scanning Calorimetry

MATERIALS FOR SEPARATIONS

155. **NOVEL MODIFIED ZEOLITES FOR ENERGY-EFFICIENT HYDROCARBON SEPARATIONS**
$218,295
DOE Contact: Sara Dillich (202) 586-7925
Sandia National Laboratories contact: T. M. Nenoff (505) 844-0340

The purpose of this research is to develop a new class of inorganic zeolite based membranes for light gas separation and use this technology to improve on separation efficiencies currently available with polymer membranes, particularly for light alkanes. Components of the research include 1) the development of methods to selectively modify the sorptive properties of known zeolites 2) creation of new adsorbents by the modification of known zeolites 3) evaluation of the feasibility of adsorbent-based hydrocarbons separation processes replacing energy intensive and energy inefficient processes, and 4) the creation of the basis for a predictive model so adsorbents can be tailored for particular processes. The approach is to determine zeolite type and carbon source relationships, industrial plant testing, and engineering analysis and feedback.

Keywords: Coatings, Sol-Gel Processing, Membranes, Separations, Zeolite

MATERIALS FOR ENGINEERING COMPONENTS

156. **ADVANCED CHLOR-ALKALI TECHNOLOGY**
$600,000
DOE Contact: Sara Dillich (202) 586-7925
Los Alamos National Laboratory contact: Jerzy Chlistunoff (505) 667-7192

The aim of this project is to develop a process to replace the hydrogen-evolving cathode in chlor-alkali cells with an oxygen-consuming cathode and thus reduce the electrochemical cell voltage. The original cathode hardware was replaced by fuel cell type hardware to eliminate membrane delamination and extend cell lifetime. Modifications of the cathode hardware also resulted in significant improvement of cell performance. Project accomplishments include: (i) three months of stable cell operation at a throughput 2.5 times higher than the industry standard (ii) improvement and stabilization of caustic current efficiency at around 90% at high throughputs, and (iii) reduced generation of unwanted by-product peroxide. Anticipated further improvements of the cell structure and its operating conditions should bring the technology to the point where it will become attractive for industry to invest in its scale-up and implementation.

Keywords: Electrochemical Cell, Oxygen Consuming Cathode

157. **DEVELOPMENT AND DEMONSTRATION OF ADVANCED TOOLING ALLOYS FOR MOLDS AND DIES**
$480,000
DOE Contact: Sara Dillich (202) 586-7925
Idaho National Engineering and Environmental Laboratory Contact: Kevin McHugh, (208) 525-5713

The goal of the project is to research, develop, and demonstrate a new class of tooling alloys that improve productivity, increase die life, and at the same time, reduce the energy consumed during the production of dies used in glass component manufacture, forging, die casting, and stamping. Tool steel samples were prepared by spray forming, a rapid solidification processing method. These samples were tempered and the microstructure and hardness are being analyzed.

Keywords: Tool Steel, Molds, Glass, Forging, Die Casting, Heat Treating, Rapid Solidification, Spray Forming

158. **STRESS-ASSISTED CORROSION IN BOILER TUBES**
$276,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The goal of this project is to clarify the mechanisms of stress assisted corrosion (SAC) of boiler tubes for determining key parameters in its mitigation and control. The centerpiece of this R&D is the development of a laboratory test that 1) simulates SAC in industrial boilers and 2) permits the control of key conditions to establish the parameters that have the greatest effects on SAC initiation and propagation. The R&D partners and industry contributors will use information gathered across multiple industries, make in situ measurements of strain and water chemistry in operating boilers, and perform laboratory simulations of SAC. Through these activities, significant environmental, operational, and material characteristics are being identified to select parameters for each that reduces the frequency and severity of SAC. In addition, risk factors for SAC are being identified to determine inspection intervals and priorities for control. It is anticipated that the results will yield increased operating efficiencies represented by decreased downtime (greater intervals between inspection and maintenance cycles) with associated energy and cost savings.

Keywords: Stress Assisted Corrosion, Tubes, Industrial Boilers, Strain and Water Chemistry

159. **VIRTUAL WELDED-JOINT DESIGN INTEGRATING ADVANCED MATERIALS AND PROCESSING TECHNOLOGIES**
$100,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The primary goal of this project is to use an integrated modeling approach to increase weld joint service performance by 10 times and to reduce energy use by 25 percent through performance and productivity improvements. This integrated model will address base material selection, weld consumable design, welding process parameters optimization, weld residual stress management, and fatigue resistance improvement. The project will integrate existing modeling tools with new enhancements to develop a systematic microstructure-level modeling approach for the design of a high-performance weld joint. The systematic modeling approach will lead to an optimized weld joint design by considering the combined effects of weld bead geometry, microstructure, material property, residual stress, and the final fatigue strength. The computer–aided virtual weld joint design will also enable improvement of the manufacturing quality, resulting in increased manufacturing productivity and reduced energy consumption for welding and reduced welding emissions.

Keywords: Welding, Advanced Materials, Modeling, Fatigue

160. **HIGH-PERFORMANCE, OXIDE-DISPERSION-STRENGTHENED TUBES FOR PRODUCTION OF ETHYLENE AND OTHER INDUSTRIAL CHEMICALS**
$185,278
DOE Contact: Sara Dillich (202) 586-7925

This project seeks to develop higher-temperature creep resistant and coking-resistant tubes for ethylene pyrolysis and steam methane reforming. Oxide-dispersion strengthened (ODS) tubes are expected to have high creep resistance, exhibit substantial fabricability, and show environmental benefits. Project partners are developing tubes from iron, nickel aluminide, and advanced metallic alloy materials resistant to the coking and carburization that plague traditional tubes of cast or wrought high-alloy stainless steel. These novel tubes are expected to allow an increase of 65˚C in tube operating temperature during ethylene production and a doubling of time between decoking cycles at equivalent temperature. The specific objective is to develop a clad INCOLOY™ Alloy MA 956/ODS Alloy 803 tubing that exhibits up to a factor of 2 improvement in creep strength and coking resistance compared with current alloys. Experimental tubes have been fabricated by extrusion and are being evaluated.

Keywords: Alloys, Furnace Tubes, Dispersion Strengthening, Ethylene, Industrial Chemicals, Creep Resistance, Coking, Metals, Welding

161. **NOVEL CARBON FILMS FOR NEXT GENERATION ROTATING EQUIPMENT APPLICATIONS**
$209,709
DOE Contact: Sara Dillich (202) 586-7925

This project aims to combine the unique qualities of two novel carbon technologies to achieve extended wear life and higher energy savings in rotating-equipment applications, including mechanical seals, sliding bearings, and shafts. Materials to be explored in this project are a super low-friction carbon film [Near Frictionless Carbon (NFC)] and a carbon conversion film with structure and properties ranging from graphite to diamond [Carbide Derived Carbon (CDC)]. The focus of the R&D is the development of adherent, low-friction, wear-resistant coatings for SiC and other metal carbide ceramics for rotating seal applications. Activities will include treating SiC components to produce CDC surface layers, characterizing the coatings and substrates, and evaluating of coated components tested in the laboratory and in industry. NFC coatings will be applied to both untreated and CDC-treated components.

Keywords: Carbon Materials, Rotating Equipment, Coatings, Ceramics, SiC, Friction, Near Frictionless Carbon, Carbide Derived Carbon

162. **PHYSICAL AND NUMERICAL ANALYSIS OF EXTRUSION PROCESS FOR PRODUCTION OF BI-METALLIC TUBES**
$175,315
DOE Contact: Sara Dillich (202) 586-7925

The primary project objective is to understand and control metal flow in the coextrusion of bimetal tubes. Two metals will be selected based on their service properties, such as corrosion resistance, elevated-temperature performance, strength, ductility, and surface finish. Process parameters such as temperature, ram speed, extrusion ratio, and lubrication on both container and mandrel interfaces with the extruded billet, will be included in the final model. One objective of this newly developed numerical model will be to indicate a selection of extrusion press characteristics (e.g., press capacity, container size) based on the required bimetal tube specifications. Tests are being performed to determine if the amount of deformation in the process plays a significant role in the development of the microstructure between the two materials, bond integrity, and dimensional stability. The deformation is being modeled by finite element techniques.

Keywords: Tubes, Metals, Numerical Modeling, Finite Element Modeling, Billet, Extrusion, Corrosion Resistance

OTHER

163. **METALS PROCESSING LABORATORY USERS (MPLUS) FACILITY**
$1,350,000
DOE Contact: Sara Dillich (202) 586-7925
ORNL Contact: Peter Angelini (865) 576-8069

The Metals Processing Laboratory User (MPLUS) Facility is an officially designated DOE User Facility. It's primary focus is related to the Office of Industrial Technologies (OIT) efforts including the "Industries of the Future", national, and cross cutting prograMs. The purpose of MPLUS is to assist U. S. industry and academia in improving energy efficiency and enhancing U. S. competitiveness. MPLUS includes the following user centers: Metals Processing, Metals Joining, Metals Characterization, and Metals Process Modeling. As of the end of FY 2001, 0ver 160 proposals were received with over 60 MPLUS projects having been completed. Projects crosscut all of the industries in the Industries of the Future effort and other supporting industries including forging, heat treating, welding.

Keywords: Industry, User Center, Metals, Materials, Processing, Joining, Properties, Characterization, Modeling, Process, Welding

SOLAR ENERGY TECHNOLOGY PROGRAM

	FY 2003
SOLAR ENERGY TECHNOLOGY PROGRAM - GRAND TOTAL	$26,623,000
NATIONAL PHOTOVOLTAICS PROGRAM	$26,623,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$13,655,000
Amorphous Silicon for Solar Cells and Polycrystalline Thin-Film Materials for Solar Cells	11,973,000
Film Silicon for Solar Cells	522,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	455,000
Nanocrystalline Solar Cell Materials	299,000
Organic Solar Cell Materials	406,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$10,058,000
Materials and Device Characterization	6,007,000
Materials Structure and Composition	4,051,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,910,000
Materials Improvement for High-Efficiency Crystalline Silicon Solar Cells	580,000
Instrumentation and Facilities	2,330,000

SOLAR ENERGY TECHNOLOGY PROGRAM

OFFICE OF SOLAR ENERGY TECHNOLOGIES

The National Photovoltaics Program sponsors research and development with the goal of making terrestrial solar photovoltaic power a significant and commercially viable part of the national energy mix. From such efforts, private enterprise can choose options for further development and competitive application in U.S. and foreign electric power markets. Approximately 70 percent of the U.S. domestic product is exported to developing countries. The objective of materials research is to overcome technical barriers that limit the efficiency and cost effectiveness of photovoltaic cells. Conversion efficiency of photovoltaic cells is limited by the spectral response of the semiconductor (dependent on band structure), carrier mobility, and device engineering factors. These factors include junction depth, reflection coefficient, parasitic resistances (i.e., series resistance in the metallization and contacts, shunt resistance through the thickness of the cell), and material imperfections that support dark recombination of excess photogenerated carriers. Manufacturing cost is affected by the expense of semiconductor material growth, the complexity of junction formation and cell fabrication, and the material requirements of final module assembly. While most photovoltaics in the U.S. have (historically) been intended for remote stand-alone applications, an increasing number of domestic deployments are intended for a grid-tied (net metering) environment. World-wide photovoltaic module production in CY 2003 is estimated at 740 MW, with about 127 MW made in the U.S.

NATIONAL PHOTOVOLTAICS PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

164. **AMORPHOUS SILICON FOR SOLAR CELLS and POLYCRYSTALLINE THIN-FILM MATERIALS FOR SOLAR CELLS**
$11,973,000
DOE Contact: Jeffrey Mazer: (202) 586-2455
NREL Contacts: Ken Zweibel (303) 384-6441,
Bolko von Roedern (303) 384-6480 and
Harin Ullal (303) 384-6486

Amorphous Silicon: These projects perform research on the deposition and characterization of amorphous silicon thin films to improve solar cell conversion efficiency and high-throughput manufacturability. Efficient conversion is hindered by the well-known, but still unresolved, light degradation effect characteristic of amorphous silicon PV devices, i.e., Staebler-Wronski Effect. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition, and sputtering. The long term goal is to develop technology for 15 percent efficient (stabilized) photovoltaic modules with cost under $\$50/m^2$ and with 30-year lifetime. This will allow system lifetime energy cost under $0.06/kWh, and subsequent wide competition of amorphous Si-based PV in large-scale distributed power scenarios.

Polycrystalline Thin Films: These projects perform applied research on the deposition of $CuIn(Ga,S)Se_2$ (CIGSS) and CdTe polycrystalline thin films for solar cells. Research is focused on improving conversion efficiency by depositing more nearly stoichiometric CIGSS and CdTe films, by controlling interlayer diffusion and lattice matching in heterojunction structures, by thinning the CdS window layer to under 0.1 microns, and by controlling the uniformity of deposition over large (4000 cm^2) areas. The films can be deposited by chemical and physical vapor deposition, by electrodeposition, and by sputtering. The long term goal is to develop technology for 15 percent efficient photovoltaic modules with cost under $\$50/m^2$ and with 30-year lifetime. This will allow system lifetime energy cost under $0.06/kWh, and subsequent wide competition of polycrystalline film-based PV in large-scale distributed power scenarios.

Keywords: Amorphous Silicon, Amorphous Materials, Polycrystalline Films, Copper Indium Diselenide, Cadmium Telluride, Coatings and Films, Chemical Vapor Deposition, Sputtering, Physical Vapor Deposition, Electrodeposition, Semiconductors, Solar Cells

165. **FILM SILICON FOR SOLAR CELLS**
$522,000
DOE Contact: Jeffrey Mazer (202) 586-2455,
NREL Contacts: Ken Zweibel (303) 384-6441and
Harin Ullal (303) 384-6486

These projects perform applied research on the high-throughput deposition of relatively thin crystalline silicon (50-100 microns). Methods include recrystallization of silicon powder on inexpensive ceramic substrates, and are amenable to rapid thermal annealing (RTA) and integrated module manufacturing techniques. The goal is to develop highly cost effective crystalline silicon modules, with conversion efficiencies in the 12-14 percent range.

Keywords: Crystalline Silicon, Film Silicon, Silicon Recrystallization, Rapid Thermal Annealing, Semiconductors, Solar Cells

166. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$455,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Sarah Kurtz (303) 384-6475,
Martha Symko-Davies (303) 384-6528 and
Robert McConnell (303) 384-6419

These projects perform research on the deposition and conduction properties of III-V semiconductors for super high efficiency concentrator solar cells. Research is focused on precise deposition of layers, elucidation of the properties of the interfacial regions, selection of manufacturable combinations of lattice-matched (and also lattice-mismatched) materials with appropriate bandgaps, and improved understanding of the conduction limiting mechanisms of the materials. Conduction limiting mechanisms are particularly severe in the case of GaInAsN, an otherwise favorable material for use in a four-junction super high efficiency concentrator cell. The materials are deposited by metal organic chemical vapor deposition, liquid phase epitaxy, and molecular beam epitaxy. The long-term goal is to develop three- and four-junction III-V-based cells that achieve as much as 40 percent efficiency under high-ratio concentration.

Keywords: Gallium Arsenide, III-V Materials, High-Efficiency Solar Cells, MOCVD, MBE, Liquid-Phase Epitaxy, Semiconductors, Ternary Semiconductors, Quaternary Semiconductors, Solar Cells, Concentrator Cells

167. **NANOCRYSTALLINE SOLAR CELL MATERIALS**
$299,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Dave Ginley (303) 384-6573 and
Art Nozik (303)-384-6603

These projects focus on the development of nanocrystalline films (including dye-sensitization of nanocrystalline films of titanium dioxide), photovoltaic devices based on nanocrystal composites, nanostructure arrays for multi-junction solar cells, and biomemetic films employing semiconductor nanocrystal composites. This fundamental research explores the physical mechanisms, and identifies the limits to efficiency and future commercial viability, of these materials.

Keywords: Nanocrystalline Films, Nanostructures, Dye-Sensitized Cells, Nanocrystals, Biomemetics

168. **ORGANIC SOLAR CELL MATERIALS**
$406,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Robert McConnell (303) 384-6419

These projects explore the physics and chemistry of next-generation organic-based materials which have a potential for efficient and low-cost solar energy conversion. Projects include liquid-crystal based solar cells, polymer hybrid photvoltaics, ordered molecular light harvesting arrays, and double heterostructure and tandem organic solar cells.

Keywords: Organic Solar Cells, Polymer Solar Cells, Conductive Polymers, Next-Generation Photovoltaics

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

169. **MATERIALS AND DEVICE CHARACTERIZATION**
$6,007,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Pete Sheldon (303) 384-6533

These projects measure and characterize material and device properties. Approaches include surface and interface analysis, compositional analysis, electro-optical characterization, and cell performance and material evaluation. These allow study of critical material/cell parameters such as impurities, layer mismatch, and other defects that limit photovoltaic performance and lifetime. Specific techniques include deep level transient spectroscopy, electron beam induced current, secondary ion mass spectroscopy, x-ray photoelectron spectroscopy, scanning electron microscopy and scanning transmission electron microscopy, Auger spectroscopy, Fourier-transform based measurements (e.g., FT-Raman, FTIR, and FT-PL), radio-frequency photoconductive decay, ellipsometry, and photoluminescence.

Keywords: Nondestructive Evaluation, Surface Analysis, Surface Characterization, Semiconductor Microstructure, Analytical Microscopy, Minority Carrier Lifetime Measurement, Semiconductor Defects, Solar Cell Testing, Module Testing

170. **MATERIALS STRUCTURE AND COMPOSITION**
$4,051,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Alex Zunger (303) 384-6672,
John Benner (303) 384-6496 and
Robert McConnell (303) 384-6419

These projects support the fundamental and exploratory research needed for advancement of PV technologies in the long term—five to ten years—and beyond. Projects include collaboration with Office of Science (SC). Topics include ordering in ternary and quaternary materials, solid state spectroscopy, solid state theory of photovoltaic semiconductors, computational material sciences, structure of photoelectrochemical materials such as dye-sensitized solar cell materials, properties of transparent conducting oxides, structure of GaInAsN alloys, impurity precipitation and dissolution in crystalline silicon, and structure of hydrogen incorporation in silicon materials.

Keywords: Semiconductor Structure, Solid State Spectroscopy, Ordering in Semiconductors, Photoelectrochemical Materials, Semiconductor Defects, Crystalline Defects, Semiconductor Impurities, Quaternary Semiconductors, Nanostructured Materials

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

171. **MATERIALS IMPROVEMENT FOR HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS**
$580,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: John Benner (303) 384-6496

This project performs applied research on crystalline silicon materials and devices to improve conversion efficiency in a commercially-compatible process. Methods employ advanced back-surface fields and silicon nitride and other bulk passivation treatments to reduce minority carrier recombination at cell surfaces and in the bulk. Control of point defects in crystalline silicon is studied by a variety of techniques, and is thoroughly discussed at the NREL-sponsored Silicon Devices and Materials Conference held in Colorado each August. Much work is done at the DOE Center of Excellence in Photovoltaics at Georgia Institute of Technology. One of the major goals of this project is to develop a rapid-thermal-processing (RTP)-based, screen-printed-contact, photolithography-free protocol that will yield 18 percent efficient 100 cm^2 cells on crystalline material. Crystalline silicon materials for achieving this goal include multicrystalline silicon made by the Heat Exchange Method (HEM), ribbon material, and single-crystal silicon made by the Czochralski growth method.

Keywords: Crystalline Silicon, Multicrystalline Silicon, High-Efficiency Silicon Cell, Screen Printing Metallization, Light Trapping, Back-Surface Field, Rapid Thermal Processing, Crystalline Silicon Defects, Point Defects, Hydrogen Passivation, Silicon Nitride Passivation, Heat Exchange Method (HEM), Silicon Ribbon

172. **INSTRUMENTATION AND FACILITIES**
$2,330,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Larry Kazmerski (303) 384-6600 and Pete Sheldon (303)384-6533

This project includes equipment procurement and staff support for the measurement and characterization of photovoltaic materials and devices. Typical equipment includes those for such measurements as ellipsometry, Auger analysis, current-voltage characteristic, Fourier transform-based spectroscopy, and electron microscopy; and film growth equipment such as MBE, ECR plasma, and sputtering systems for the fabrication of photovoltaic and related materials, and ancillary materials used with this equipment.

Keywords: Semiconductor Measurement Equipment, Semiconductor Materials Measurement, Semiconductor Characterization, Fourier Transform Spectroscopy, Solar Cells, Electron Microscopy, MBE, MOCVD

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM

	FY 2003
WEATHERIZATION & INTERGOVERNMENTAL PROGRAM - GRAND TOTAL	$0
FINANCIAL ASSISTANCE PROGRAM	$0
INVENTIONS AND INNOVATION (I&I)	$0
Ceramic Composite Die for Metal Casting	0[9]
Foamed Recyclables	0[1]
Weldcomputer[tm] Resistance Welder Adaptive Control	0[1]
Development of a Composite Reinforced Aluminum Conductor	0[1]
Environmental Tensometer	0[1]
Frequency-selective Solar Glazing System	0[1]
High-intensity Silicon Vertical Multi-junction Solar Cells	0[1]
High-temperature Coating for Gas Turbines Components	0[1]
High-temperature Refractory Ceramic	0[1]
improved Methods to Manufacture Carbon-alumina Composite Anodes for Aluminum Reduction	0[1]
Manufacturing Ceramic Products from Waste Glass	0[1]
Membrane Technology to Remove Entrapped Air from Ammonia Refrigeration Systems	0[1]
Nickel-based Superalloy with Improved Weldability and Oxidation Resistance	0[1]
Novel Technique for Increasing Corrosion Resistance of Aluminum and Aluminum Alloys	0[1]
Phosphors for Use in High-efficiency Lighting and Displays	0[1]
Self-dressing Resistance Welding Electrode	0[1]
Titanium Matrix Composite Tooling Material for Aluminum Die Castings	0[1]
Tough-coated Hard Powders (TCHP)	0[1]
Tribopolymerization as an Anti-wear Mechanism	0[1]
Wear Resistant Composite Structure of Vitreous Carbon Containing Convoluted Fibers	0[1]
A Hot Eye[tm]-based Coordinate Measuring Machine for the Forging Industry	0[1]
Cupola Furnace Computer Process Model	0[1]
Development of a High-frequency Eddy-current Separator	0[1]
Direct Pour In-mold (DPI) Technology for Producing Ductile and Compacted Graphite Iron Castings	0[1]
High Energy-density Double-layer Capacitor Energy Storage for Pv Systems	0[1]
Insoluble Titanium-lead Anode for Sulfate Electrolytes	0[1]
Lightweight and Cost-effective Cast Aluminum Diesel Engine Head with Localized Reinforcement	0[1]
Lost Foam Casting Quantifier Program	0[1]
A Viable Inert Cathode for Smelting Primary Aluminum	0[1]
Batch Preheat for Glass and Related Furnace Processing Operations	0[1]
Brazing and Spot Welding Innovations for Joining Aluminum Alloys	0[1]
Composite Electrodes for Advanced Electrochemical Applications	0[1]
Development of Aluminum-iron Alloys for Magnetic Applications	0[1]
Development of Inert Anode for the Primary Aluminum Industry	0[1]
Energy Saving Lightweight Refractory	0[1]
Fabrication and Testing of a Prototype Ceramic Furnace Coil	0[1]
Germanium Compounds as Highly Selective Fluorination Catalysts	0[1]
Highly Efficient Rapid Tooling Using Optimized Cooling Passages	0[1]
Low-energy Alternative to Commercial Silica-based Glass Fibers	0[1]
Novel Ceramic Composition for Hall-Héroult Cell Anode Application	0[1]

[9] Prior year funding

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM (continued)

	FY 2003
FINANCIAL ASSISTANCE PROGRAM (continued)	
NICE³ TECHNOLOGIES	$0
Die Casting Copper Motor Rotors	0[1]
Microsmooth Process on Aluminum Wheels	0[1]
Process to Recover and Reuse Sulfur Dioxide in Metal Casting Operations	0[1]
Processing Electric Arc Furnace Dust into Saleable Chemical Products	0[1]
Rapid Heat Treatment of Cast Aluminum Parts	0[1]
Commercial Demonstration of an Improved Magnesium Thixomolding Process	0[1]
Improvement of Lost Foam Casting Process	0[1]
Non-vacuum Electron Beam Welding	0[1]
Vanadium Carbide Coating Process	0[1]

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM

FINANCIAL ASSISTANCE PROGRAM

INVENTIONS AND INNOVATION (I&I)

The U.S. Department of Energy's (DOE's) Inventions and Innovation (I&I) program is specifically for individuals or small businesses, for whom developing an energy-saving invention can be difficult. I&I offers financial and technical support to inventors and businesses for promising energy-saving concepts and technologies. I&I selects technologies to receive grants through a competitive process. Inventors can apply for a grant when I&I releases an announcement of funding opportunity. Technologies that offer significant energy savings and future commercial market potential are eligible for I&I support.

I&I provides financial assistance for research and development of innovative, energy-savings ideas and inventions. This assistance is provided at three levels: Up to $50,000 for technologies in early-stage development, up to $250,000 for technologies approaching the point of prototype, and up to $500,000 for technology demonstrations. Cost-share is strongly encouraged to receive a Category 1 or 2 award, and cost-share is required to receive a Category 3 award.

In addition to competitively awarded financial assistance, I&I offers its grantees technical guidance through mentoring, and access to information through technology events and referrals. Publications and a database of inventor resources are available to the public at http://www.eere.energy.gov/inventions/energytechnet/.

173. **CERAMIC COMPOSITE DIE FOR METAL CASTING**
$0[10]
DOE Contact: Lisa Barnett (202) 586-2212
MER Corporation Contact: James Withers (520) 574-1980

Materials and Electrochemical Research (MER) Corporation has developed and is now selling ceramic composite material that is used as casting dies. Ceramic composite materials offer complete stability to molten metals and are resistant to erosion, oxidation, thermal fatigue, and cracking. The potential life span of ceramic composite dies is five to ten times that of coated steel dies.

Keywords: Die Casting, Ceramic Composite, Metal Casting

174. **FOAMED RECYCLABLES**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Century-Board USA Contact: Wade Brown (714) 871-5580

Century-Board USA, a licensee of Ecomat, Inc., has a fully developed process to convert solid wastes into synthetic building materials. The process consists of mixing up to 85 percent solid waste into a modified polyester polyurethane resin with special additives. This polymer system is a thick liquid that is poured into discrete molds or continuously cast, as is done with the 'plastic' lumber. This thick liquid then forms and fills all the crevices of the mold and produces a lightweight, hard, and tough product. The material does not contain thermoplastics such as polyethylene or PVC, wood or sawdust unless requested by the customer.

Keywords: Synthetic Lumber, Solid Waste Recycling

175. **WELDCOMPUTER™ RESISTANCE WELDER ADAPTIVE CONTROL**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
WeldComputer Corp. Contact: Dennis Hull (518) 283-2897

WeldComputer Corporation developed and is selling a sophisticated computer-controlled resistance welding system designed particularly for resistance spot welding. The WeldComputer system consists of a programmable power controller, line voltage monitoring and compensation equipment, and other sensors and compensation equipment that monitor the welding process and make real-time adjustments. The technology is less energy intensive than other metal-joining methods through precise control of electric current. The new L-Series systems are affordable and have tremendous potential for use in the automotive, appliance, and other industries.

Keywords: Welding, Process Control System

[10]Prior year funding

176. **DEVELOPMENT OF A COMPOSITE REINFORCED ALUMINUM CONDUCTOR**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
W. Brandt Goldsworthy and Associates, Inc. Contact:
Mike Winterhalter (310) 375-4565

W. Brandt Goldsworthy and Associates is working to commercialize an automated, high-throughput manufacturing method capable of producing a composite-reinforced aluminum conductor reliably and at a cost competitive with conventional conductors. The use of composite materials in utility transmission and distribution lines promises substantial, long-term cost and weight benefits.

Keywords: Aluminum Conductors, Transmission and Distribution Lines

177. **ENVIRONMENTAL TENSOMETER**
$0[11]
DOE Contact: Lisa Barnett (202) 586-2212
Penn State University Contact: Richard Tressler
(814) 865-7961

Researchers at Penn State have developed and are using a device for high temperature testing of the tensile strength and related physical properties of single-filament refractory fibers under varying atmospheric conditions, new small composites, and thin membranes for oxygen separation applications. The system integrates a furnace, testing unit, gas-handling system, vacuum system, and PC-based software.

Keywords: Materials Testing, High Temperature Material Properties

178. **FREQUENCY-SELECTIVE SOLAR GLAZING SYSTEM**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Orion Engineering, Inc. Contact: Thomas Regan
(978) 589-9850

Orion Engineering is developing a novel frequency-selective glass material for use in automobile, building, or solar-thermal collector application. This material is capable of transmitting selective frequencies of light with almost no reflection while efficiently transmitting visible light. The glazing could be used to minimize direct solar heating, resulting in reduced heating and cooling requirements for buildings and automobiles.

Keywords: Glazing, Windows, Frequency-Selective Glass

179. **HIGH-INTENSITY SILICON VERTICAL MULTI-JUNCTION SOLAR CELLS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
PhotoVolt, Inc. Contact: Bernard Sater
(440) 878-1073

PhotoVolt, Inc. has developed a low-cost, high-volume fabrication process for high intensity vertical multi-junction (VMJ) solar cells and is demonstrating the cell's performance viability in solar concentrators. The unique features of the VMJ cell make it capable of more efficient operation at higher intensities than other silicon concentrator solar cell designs. Prototype testing is finished and orders are being taken for the new VMJ cell.

Keywords: Solar Cells, Solar Concentrators, Photovoltaic

180. **HIGH-TEMPERATURE COATING FOR GAS TURBINES COMPONENTS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Turbine Coatings, Inc. Contact: Maggie Zhing
(518) 348-0551

Turbine Coatings, Inc. is developing a new coating with cracking resistance and enhanced oxidation protection for hot section components of gas turbines. Energy savings will be derived from reducing one of the two traditional coating steps and extending component life.

Keywords: Coatings, Gas Turbines

181. **HIGH-TEMPERATURE REFRACTORY CERAMIC**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Trilliam Thermo Technologies Contact:
Charles Flanagan (541) 426-6021

Trilliam Thermo Technologies is developing a new castable refractory liner material to be used in high temperature rotary kilns.The capabilities of this new ceramic liner will be a 200˚C improvement in maximum allowable operating temperatures, an operating life extension of five times, and additional cost savings in installation.

Keywords: Refractory Ceramic, Rotary Kiln

[11]Prior year funding

182. **IMPROVED METHODS TO MANUFACTURE CARBON-ALUMINA COMPOSITE ANODES FOR ALUMINUM REDUCTION**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Golden Northwest Aluminum Co. Contact:
Alan Barkley (541) 298-0864

Golden Northwest Aluminum Company is testing a prototype improved metallic anode for electrochemically reducing aluminum. The anode obviates the need for using carbon and makes it possible to operate the cell at a lower temperature. The process produces oxygen instead of carbon dioxide and perfluorocarbon emissions.

Keywords: Aluminum Reduction, Metallic Anode

183. **MANUFACTURING CERAMIC PRODUCTS FROM WASTE GLASS**
$0[12]
DOE Contact: Lisa Barnett (202) 586-2212
Haun Labs Contact: Michael Haun (707) 538-0584

Ceramic products have traditionally been processed from raw materials that require high firing temperatures and energy-intensive processing steps. Haun Labs has developed and is now marketing a new process that lowers energy costs by substituting raw materials with recycled container-glass waste. Products manufactured by this new method are less sensitive to contaminants in the glass and can be made from difficult-to-recycle green or mixed-color waste glass. Firing temperatures can be reduced by as much as 37 percent, lowering energy costs and CO_2 emissions.

Keywords: Glass Recycling, Ceramic Tiles

184. **MEMBRANE TECHNOLOGY TO REMOVE ENTRAPPED AIR FROM AMMONIA REFRIGERATION SYSTEMS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Enerfex, Inc. Contact: Richard Callahan
(802) 658-6629

Enerfex, Inc. has developed and tested an ammonia-selective gas separation membrane technology to determine operating parameters. The technology is potentially a simplified way to continuously purge air from ammonia refrigeration plants. A prototype commercial membrane separator is proposed for evaluation in an ammonia refrigeration test skid.

Keywords: Ammonia Refrigeration, Air Purging

185. **NICKEL-BASED SUPERALLOY WITH IMPROVED WELDABILITY AND OXIDATION RESISTANCE**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Penn State University Contact: Eric Whitney
(814) 865-3916

Researchers at Penn State have completed testing of a new nickel-based superalloy. Oxidation resistance was shown to be equivalent to current-generation single crystal alloys, and weldability was determined to be excellent without the need for preheating. The alloy derives its' properties by the addition of palladium, which enhances high-temperature oxidation resistance and allows for a reduction in aluminum that directly results in improved weldability. The major application would be for the repair of turbine blades.

Keywords: Nickel-Based Superalloy, Turbine Blades

186. **NOVEL TECHNIQUE FOR INCREASING CORROSION RESISTANCE OF ALUMINUM AND ALUMINUM ALLOYS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Ohio State University Contact: Rudolph Buchheit
(614) 292-6085

Researchers at Ohio State U. have developed a new process that imparts a corrosion-resistant coating to aluminum and aluminum alloys. The process uses nontoxic lithium and magnesium salts, with or without heat treatment, to replace the currently used hexavalent chromium, which is known to be a highly toxic carcinogen. This process can be used to protect any aluminum product such as siding, cans, airplane parts, etc.

Keywords: Corrosion Resistance, Aluminum Products

187. **PHOSPHORS FOR USE IN HIGH-EFFICIENCY LIGHTING AND DISPLAYS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212 Brilliant Technologies, Inc. Contact: Douglas Kezler
(541) 737-6736

Brilliant Technologies, Inc. has developed new phosphors for use in high-efficiency, LED-activated lamps and displays, providing improved color rendering and significant energy savings. The phosphors will provide for the first time a means to produce true tri-chromatic white light under LED excitation.

Keywords: Phosphors, LED-Activated Lamps, LED

[12]Prior year funding

188. **SELF-DRESSING RESISTANCE WELDING ELECTRODE**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Lektrocorp, Inc. Contact: Bryan Prucher (313) 974-3137

Lektrocorp designed, tested and produced an electrode from a unique metal-matrix composite material that employs a ceramic substrate as the load-bearing element and a metal matrix as the conduit for the electric current flow. The project was carried out in four separate tasks, consisting of material selection, design development and optimization, fabrication and model verification, and performance testing and evaluation. This new electrode would replace the conventional welding electrode in auto manufacturing.

Keywords: Resistance Welding Electrode, Auto Manufacturing

189. **TITANIUM MATRIX COMPOSITE TOOLING MATERIAL FOR ALUMINUM DIE CASTINGS**
$0[13]
DOE Contact: Lisa Barnett (202) 586-2212
Dynamet Technology, Inc. Contact: Susan Abkowitz (781) 272-5967

Dynamet Technology, Inc. produced and is now testing a metal matrix composite material composed of Ti-6Al-4V and 10 wt% titanium carbide particulate for aluminum die casting. The titanium metal matrix composite offers both dramatically improved (400 percent) durability and reduced thermal conductivity (50 percent compared to steel) which will provide energy savings by reducing preheating energy consumption by 4-8 percent.

Keywords: Metal Matrix Composite, Titanium, Aluminum, Die Casting

190. **TOUGH-COATED HARD POWDERS (TCHP)**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Allomet Corp. Contact: Rick Toth (724) 864-4767

Allomet Corporation is developing a new process to sinter tungsten carbide particles resulting in a new class of tool and die materials. These new materials have increased hardness, strength, and abrasion resistance with the potential to extend tool life 10-25 times.

Keywords: Tungsten Carbide, Wear Resistant Tools

191. **TRIBOPOLYMERIZATION AS AN ANTI-WEAR MECHANISM**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Virginia Polytechnic Institute Contact: Michael Furey (540) 231-7193

Researchers at Virginia Polytechnic Institute are developing an advanced technology called tribopolymerization that uses molecules called monomers to create perpetually renewing films directly on surfaces that require lubrication, such as ceramic or alloy steel. Unlike the action of surface treatments of coatings, which wear away, these protective polymeric films form continuously in critical areas of boundary lubrication and wear. The films efficiently form in localized areas where the greatest amount of wear occurs, reducing wear and friction, and saving energy in the process.

Keywords: Wear Reduction, Boundary Lubrication

192. **WEAR RESISTANT COMPOSITE STRUCTURE OF VITREOUS CARBON CONTAINING CONVOLUTED FIBERS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
MRCC, Inc. Contact: Richard Ludington (919) 785-1197

MRCC, Inc has developed and is testing a novel method to make a composite material consisting of a vitreous carbon matrix containing convoluted fibers. The resulting product has better wear resistance, lower coefficient of friction and higher electrical conductivity than competing materials. The material is being developed for use in cable, motor brushes, and third rail electric transportation systems, such as light rail.

Keywords: Composite Material, Cables, Motor Brushes

193. **A HOT EYE™-BASED COORDINATE MEASURING MACHINE FOR THE FORGING INDUSTRY**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
OG Technologies Contact: Dr. Tzyy-Shuh Chang (734) 769-8500

OG Technologies is developing a 3-dimensional measurement system for the domestic forging industry based on HotEyeä. This technology will allow a high definition camera to accurately image a red hot object. The project marries conventional Coordinate Measurement Machine "CMM" technology to HotEyeä technology to permit the accurate measurement of forged parts while

[13]Prior year funding

they are at high temperature. Being able to take such measurements will dramatically reduce the amount of scrap produced by the domestic forging industry.

Keywords: Forging, HotEye™, Coordinate Measurement Machine

194. **CUPOLA FURNACE COMPUTER PROCESS MODEL**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
S. Katz Associates, Inc. Contact: Seymour Katz (248) 682-4131

S. Katz and Associates, Inc. is developing a new computer process technology to integrate the many variables involved in cupola furnace operation. The cupola is the dominant scrap-melting furnace used in scrap-iron foundries, producing two-thirds of the liquid iron needed for castings. Cupola furnace operation involves 40 or more chemical reactions and a range of physical processes, which leads to significant operating difficulties and inefficiencies, resulting in poor-quality iron, costly remediation, and scrapped metal and castings. The model is intended to better guide everyday cupola operations and cost-benefit decisions resulting in reduced energy consumption and greenhouse-gas emissions.

Keywords: Cupola Furnace, Operations Control

195. **DEVELOPMENT OF A HIGH-FREQUENCY EDDY-CURRENT SEPARATOR**
$0[14]
DOE Contact: Lisa Barnett (202) 586-2212
EMPS Corporation Contact: Stephen Smoot (801) 582-7600

EMPS Corporation is confirming prior bench scale testing of the high-frequency eddy-current separator through the successful scale-up and testing of a prototype-size unit. The engineering prototype will be demonstrated on contaminated foundry sand and on magnesium smut at a magnesium recovery facility. An initial market study and business plan will be refined based on the results of the prototype unit testing and demonstration.

Keywords: Eddy-Current, Foundry Sand, Magnesium Smut

[14]Prior year funding

196. **DIRECT POUR IN-MOLD (DPI) TECHNOLOGY FOR PRODUCING DUCTILE AND COMPACTED GRAPHITE IRON CASTINGS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Comanche Technologies, LLC Contact: Jay Hitchings (610) 269-6241

A new "Direct Pour In-Mold" (DPI) treatment technology, being developed by Comanche Technologies, LLC, produces both ductile and CGI castings by pouring a base metal directly into a specially designed container, which is inserted into a mold. Each of the various sized containers provides all of the necessary components to produce a specific amount of treated and filtered metal. The DPI containers provide energy savings of 13.3 percent over comparable treatments, increased mold yields, very high magnesium recovery, no magnesium emissions, and no post-inoculant treatment is required.

Keywords: Ductile Castings, CGI Castings

197. **HIGH ENERGY-DENSITY DOUBLE-LAYER CAPACITOR ENERGY STORAGE FOR PV SYSTEMS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Heliocentric Contact: Troy Aaron Harvey (801) 375-4243

Today, batteries are the weakest link in photovoltaic system technology, and until now there have been no other practical alternatives. Heliocentric is developing a new energy storage technology, Terrastor, designed to address the problems associated with energy storage in photovoltaic systeMs. This new type of energy storage will achieve energy densities equivalent to lead-acid batteries while dramatically improving upon round-trip energy efficiency, cycle life, available capacity, autonomy, maintenance requirements, environmental life cycle, and embodied energy. These improved characteristics promise to redefine photovoltaic system performance, reduce embodied energy, and lower photovoltaic system lifecycle cost.

Keywords: PV Systems, Energy Storage

198. **INSOLUBLE TITANIUM-LEAD ANODE FOR SULFATE ELECTROLYTES**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Electrodes International, Inc. Contact: Dr. Alla Ferdman

Electrodes International, Inc. is developing insoluble anodes for electrowinning of metals such as copper, zinc, nickel, cobalt, etc. and for electrolytic manganese dioxide production. The proposed anodes significantly reduce contamination of the products with lead and can be used at lower voltage and increased current density, resulting in higher productivity and energy savings up to 25 percent.

Keywords: Electrowinning, Anodes

199. **LIGHTWEIGHT AND COST-EFFECTIVE CAST ALUMINUM DIESEL ENGINE HEAD WITH LOCALIZED REINFORCEMENT**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Foster-Miller, Inc. Contact: Uday Kashalikar (781) 684-4125

Foster-Miller, Inc. is producing and testing a full-scale medium-duty aluminum diesel engine head casting. Successful development and insertion of suitable diesel engines to replace gasoline engines in light trucks would produce an over 50 percent improvement in fuel economy, and would lower the national transportation energy use by over 15 percent with a comparable reduction in emissions. The challenge is to produce diesel engines with performance and weight comparable to that of current gasoline engines. Specifically, to reduce the engine weight to the level specified for light trucks, the block and head will need to be made out of aluminum (rather than the current cast iron). The problem is that the aluminum castings do not have adequate mechanical properties to withstand the high loads and temperatures in certain regions of the engine block and head. Foster-Miller's approach to overcome this problem is to locally reinforce the highly loaded regions in aluminum gravity castings with metal matrix composite (MMC) materials.

Keywords: Diesel Engines, MMC Material, Aluminum Castings

200. **LOST FOAM CASTING QUANTIFIER PROGRAM**
$0[15]
DOE Contact: Lisa Barnett (202) 586-2212
Industrial Analytics Corporation Contact: Graham V. Walford (865) 482-8424

Industrial Analytics Corporation is building a prototype of a production floor machine and demonstrating its use in a casting improvement program. The industry currently relies on visual inspection of foam patterns pieces to determine quality. The casting of inferior foam patterns results in defective castings. Each defective casting represents a waste of energy. The "Lost Foam Casting Quantifier Program" sets objectives, measurable standards, and verifies them using measured data. The properties of foam patterns may then be optimized, production yield can be maximized, quality can be assured, and disputes can be minimized.

Keywords: Lost Foam Casting, Casting Optimization

201. **A VIABLE INERT CATHODE FOR SMELTING PRIMARY ALUMINUM**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
PRACSOL, LLC Contact: Robert Rapp (614) 292-6178

Research is continuing at developing sufficient experimentation to prove the feasibility of a net shape method of manufacture and the effective properties of a porous TiB_2 body suitable as an inert cathode in the in the Hall-Héroult cell.

Keywords: Aluminum Smelting, Cathode

202. **BATCH PREHEAT FOR GLASS AND RELATED FURNACE PROCESSING OPERATIONS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Energy and Environmental Resources Contact: William Fleming (765) 647-0076

Research consisted of preparing various salt eutectics in the lab: chlorides of aluminum, iron (III), sodium, calcium, and magnesium will be used in these formulations. The salts were dissolved in various proportions, and then the water was evaporated off. Melting points were then determined in a muffle furnace. The samples which had melting points in the 200-300°F range were then tested further: in these tests, the eutectic salts were subjected to high temperature exposure (up to 1800°F) in a small lab kiln. The samples were evaluated for thermal stability and corrosivity. The salts were then used on various metal alloys at up to 1800°F. Research is still continuing.

Keywords: Salt Eutectics, Glass Preheat

203. **BRAZING AND SPOT WELDING INNOVATIONS FOR JOINING ALUMINUM ALLOYS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Inovati Contact: Ralph Tapphorn (805) 571-8384

Research is continuing to develop brazing and spot welding innovations. The technology will have immediate applications with bonding aluminum in various end-use industries, including the automotive and heat exchanger industries. The brazing and spot-welding potential of the technology could replace technologies now in operation, making the use of aluminum less problematic overall.

Keywords: Brazing, Spot Welding, Aluminum Alloys

[15] Prior year funding

204. **COMPOSITE ELECTRODES FOR ADVANCED ELECTROCHEMICAL APPLICATIONS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
North Coast Crystals Contact: Chris Kovach
(216) 321-3277

Research is continuing to demonstrate the feasibility of using diamond as a corrosion-protective coating on electrodes used in electrochemical applications. A composite electrode is being developed that consists of a copper substrate, a conductive diamond coating, and a catalytic precious metal coating.

Keywords: Electrodes, Composite Materials

205. **DEVELOPMENT OF ALUMINUM-IRON ALLOYS FOR MAGNETIC APPLICATIONS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Magna-Tech P/M Labs Contact: Kenneth Moyer
(856) 786-9061

Research is continuing to develop a powder metallurgy process to admix aluminum powder with iron powder to form iron alloy magnets. Upon sintering, a liquid phase is formed with superior magnetic properties to wrought alloys. When utilized in motor applications, the weight of small motors used in today's automobile may be reduced by 15 percent and a 15-25 percent increase in motor efficiency may be realized.

Keywords: Powder Metallurgy, Aluminum Iron Alloys, Magnets

206. **DEVELOPMENT OF INERT ANODE FOR THE PRIMARY ALUMINUM INDUSTRY**
$0[16]
DOE Contact: Lisa Barnett (202) 586-2212
Energy Research Company Contact: Robert De Saro
(718) 608-8788

Research is continuing to determine the amount and purity of the aluminum produced in a bench-scale Ionic Ceramic Oxygen Generator (ICOG) inert anode experiment and to determine anode degradation. The ICOG inert anode uses a crystal lattice to transport oxygen ions from the electrolytic solution where they are oxidized to diatomic oxygen gas. For this research project, the ICOG inert anode will replace the traditional consumable carbon anode.

Keywords: Anodes, Aluminum Production

207. **ENERGY SAVING LIGHTWEIGHT REFRACTORY**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212 Silicon Carbide Products, Inc. Contact: Mark Witmer
(607) 562-8599

Research is continuing to develop a new manufacturing technique to produce a unique silicon carbide based material that has high strength, increased high temperature qualities, and will cost less to manufacture. In addition, the new material has shown great promise in molten aluminum applications.

Keywords: Refractory, Silicon Carbide

208. **FABRICATION AND TESTING OF A PROTOTYPE CERAMIC FURNACE COIL**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
FM Technologies, Inc. Contact: Samar Guharay
(703) 961-1052

Research is continuing to demonstrate a process for joining pairs of ceramic tubes to fabricate furnace coils for ethylene production plants. Ethylene has the greatest annual production of any organic chemical and is the number one consumer of energy in the petrochemical industry. Replacement of metal alloy coils with ceramic coils could increase ethylene production by up to 10 percent leading to substantial energy savings and increased productivity.

Keywords: Ceramic Tubes, Furnace Coils, Ethylene Production

209. **GERMANIUM COMPOUNDS AS HIGHLY SELECTIVE FLUORINATION CATALYSTS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Starmet Corporation Contact: Dr. Matthew Stephens
(978) 369-5410

Research is continuing to demonstrate the concept for a new, highly selective catalyst for the fluorination of hydrocarbons. This catalyst will meet the needs of the fluorocarbon industry for process simplification, for reduction in capital costs, and for the elimination of energy intensive processing steps and separation processes.

Keywords: Germanium Compounds, Hydrocarbon Fluorination, Catalyst

[16]Prior year funding

210. **HIGHLY EFFICIENT RAPID TOOLING USING OPTIMIZED COOLING PASSAGES**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Edison Materials Technology Center Contact:
Nick Cannell (330) 425-8855

A new rapid-prototyping process is continuing to be tested that improves investment-casting technology. Unlike conventional tooling processes, this new process more quickly and efficiently produces optimized cooling lines in all tooling shapes and sizes, increasing thermal efficiency and leading to better cycle times and increased productivity. This technology has applications in the die casting and permanent mold casting industries, where problems associated with poor thermal conductivity in materials are a concern.

Keywords: Investment Casting, Die Casting, Permanent Mold Casting

211. **LOW-ENERGY ALTERNATIVE TO COMMERCIAL SILICA-BASED GLASS FIBERS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
MO-SCI Corporation Contact: Tod Neidt
(573) 364-2338

Research is continuing on developing high strength, iron phosphate glass fibers for composites and other products in the transportation, aircraft, and chemical industries. Iron phosphate glasses have a chemical durability that exceeds many commercial silica-based glasses and can be melted 3 to 20 times faster at temperatures 400-600°C lower than commercial boro-alumino-silicate glass.

Keywords: Glass, Iron Phosphate Glass Fibers, Silica-Based Glass Fibers

212. **NOVEL CERAMIC COMPOSITION FOR HALL-HÉROULT CELL ANODE APPLICATION**
$0[17]
DOE Contact: Lisa Barnett (202) 586-2212
Advanced Refractory Technologies, Inc. Contact:
Thomas Mroz (716) 875-4091

Research continues on developing a replacement for traditional carbon anodes with non-consumable material that will reduce primary aluminum production costs, reduce energy consumption by up to 20 percent, and minimize environmental impact. The research is evaluating ceramic material in anode-simulation conditions for corrosion and oxidation resistance, electrical properties, and cost efficiency compared to carbon anodes.

Keywords: Hall-Héroult, Anode, Aluminum Production

NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT, AND ECONOMICS (NICE^3)

The National Industrial Competitiveness through Energy, Environment, and Economics Program (NICE^3) is in a closeout mode. NICE^3 met its original goals to save energy, improve the environment, and provide an economic boost to U.S. industry. NICE^3 originated in 1991 as a U.S. Department of Energy (DOE) and Environmental Protection Agency (EPA) joint initiative to promote global competitiveness of U.S. iindustries through the development and commercialization of energy-efficient goods, produced with state-of-the-art energy-efficiency production technologies and practices. DOE has been the sole sponsor since 1996. NICE^3 has an excellent commercialization track record. It has resulted in the commercialization of 32 technologies, of which 27 are still on the market today. These commercial technologies have resulted in a cumulative U.S. energy savings of 34.5 trillion Btu.

213. **DIE CASTING COPPER MOTOR ROTORS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
ThermoTrex Contact: John McCoy (856) 646-5403

Traditional methods for fabricating aluminum motor rotors have been more attractive to industry because of the relatively low cost of die casting. This new technique for die casting copper motor rotors increases the life of the molds and provides a cost-effective method for producing copper motor rotor that is comparable with that for producing aluminum rotors. Copper rotors can reduce electrical motor losses by 15-20 percent, resulting in an improved efficiency that could save energy with the expanded use of copper motor rotors.

Keywords: Die Casting, Copper Motor Rotors

214. **MICROSMOOTH PROCESS ON ALUMINUM WHEELS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Metal Arts Co., Inc. Contact: Stan Dahle
(585) 546-7170

This new process is an innovative electroless nickel-plating technology that improves aluminum-chromium plating quality while substantially reducing electric and natural gas

[17] Prior year funding

usage. The new process will lower production costs and eliminate the use of zincate and the wastes associated with the traditional plating process.

Keywords: Nickel Plating, Electroless, Waste Reduction

215. **PROCESS TO RECOVER AND REUSE SULFUR DIOXIDE IN METAL CASTING OPERATIONS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Adsorption Research, Inc. Contact: Kent Knaebel (614) 798-9090

Sulfur dioxide (SO_2) is used as a catalyst in forming cold-box molds and cores in the metal casting industry. The SO_2 is typically used once, scrubbed with a caustic solution, and then discarded (flushed to sewer or sent to a waste treatment facility). This new process recovers the SO_2 for reuse by processing it through a pressure-swing absorber that is expected to recover at least 95 percent of the SO_2. Using this process will reduce energy consumption, eliminate the need for caustic effluent, and pay back costs in less than 1 year.

Keywords: SO_2 Recovery, Waste Reduction, Metal Casting

216. **PROCESSING ELECTRIC ARC FURNACE DUST INTO SALEABLE CHEMICAL PRODUCTS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Drinkard Metalox, Inc. Contact: Fred Gallagher (704) 332-8173

This unique technology will hydro-metallurgically process EAF dust into saleable products. EAF dust is oxidized and digested in acid and then treated by a series of individual steps to isolate and retrieve individual components of the dust.

Keywords: Steel Production, Waste Utilization

217. **RAPID HEAT TREATMENT OF CAST ALUMINUM PARTS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Technomics, LLC Contact: Chuck Bergman (763) 383-4720

A system that reduces 90 percent of the time and energy required to heat-treat cast aluminum components is now being demonstrated. Unlike existing technologies where components are stacked in baskets and placed in a convection or vacuum furnace, this new process uses a fluidized bed in a continuous process mode. The fluidized bed is coupled to an automated production line that moves the components through the process. Pulse-fired microprocessor-controlled burners inject heat directly into submerged radiant burner tubes, ensuring precise, even, and rapid heat transfer.

Keywords: Heat Treatment, Cast Aluminum Parts, Fluidized Bed Furnace

218. **COMMERCIAL DEMONSTRATION OF AN IMPROVED MAGNESIUM THIXOMOLDING PROCESS**
$0[18]
DOE Contact: Lisa Barnett (202) 586-2212
Thixomat, Inc. Contact: Dr. Ray Decker (734) 995-5550

Thixomat, Inc. is demonstrating the improved Thixomolding Process (semi-solid metal molding), rather than a conventional die-casting foundry operation with the objective to reduce energy usage by 50 percent, reduce scrap recycling by 50 percent, eliminate the application of global warming gas, SF_6, eliminate waste slag and dross with their disposal problems, provide a worker/ environmentally friendly process, that can be integrated into an automated manufacturing cell to produce metal and metal/plastic assemblies, and cut costs by more than 20 percent.

Keywords: Magnesium Alloy Molding, Semi-Solid Molding, Net Shape, Scrap Reduction

219. **IMPROVEMENT OF LOST FOAM CASTING PROCESS**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
General Motors Corp. Contact: Charles Gough (248) 857-2841

General Motors is evaluating and improving the Lost Foam Casting Process by applying recently developed measurement tools related to characterization of dried coating thickness and pore size distribution, improved understanding of rheology of coatings, and the ability to more accurately measure the size and shape of sand as it relates to the casting process.

Keywords: Lost Foam Casting, Metal Casting, Scrap Reduction, Sand Casting

[18]Prior year funding

220. **NON-VACUUM ELECTRON BEAM WELDING**
$0[1]
DOE Contact: Lisa Barnett (202) 586-2212
Acceleron, Inc. Contact: Don Christensen
(860) 651-9333

Electron beam welding (EBW) produces high-quality welds, but due to the vacuum requirements, is usually more expensive than conventional welding. The pieces to be welded in the EBW process must fit within a vacuum chamber, thus limiting EBW's use in high-volume production. EBW restricts the quantity and size of parts that can be welded within a pump down cycle, and requires high tooling costs to hold and manipulate multiple parts. The large diffusion pumps and mechanical pumps used to maintain the vacuum are very costly, as are the special oils required for these pumps. To address these limitations and associated costs, Acceleron Inc., is developing a plasma window that permits an electron beam, formed in a vacuum, to operate effectively and efficiently in the open air. The "window" is a stabilized gas plasma transparent to the electron beam.

Keywords: Electron Beam Welding, Non-Vacuum

221. **VANADIUM CARBIDE COATING PROCESS**
$0[19]
DOE Contact: Lisa Barnett (202) 586-2212
Metlab-Potero Contact: Mark Podob (215) 233-2600

Metlab-Potero is designing, installing, optimizing and operating a production scale system for commercial application of a vanadium carbide coating process. In addition to this, the program will develop and maintain a database for performance of the VC coatings used in different industrial applications. The database will include best practices for applications that will enable the industry to select and apply the optimum coatings.

Keywords: Vanadium Carbide, Steel, Wear Resistance, Surface Hardening

[19]Prior year funding

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

	FY 2003
OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION - GRAND TOTAL	$38,010,000
HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS	$38,010,000
Second Generation Wire Development	17,330,000
Systems Technology - Partnerships with Industry	15,650,000
Strategic Research	5,030,000

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

The Office of Electric Transmission & Distribution (OETD) is a new DOE program office formed to help ensure a robust and reliable U.S. transmission grid for the 21st century. This office combines DOE's electricity transmission and distribution (T&D) programs and research. The mission of OETD is to lead a national effort to help modernize and expand America's electric delivery system to ensure economic and national security. Broadly, that effort will include:

- reducing regulatory and institutional barriers to efficient T&D;
- acting as a neutral facilitator of solutions that benefit everyone; and
- providing a national vision for building strong public-private partnerships.

The primary functions of OETD are:

- Research and development;
- Modeling and analysis;
- Electricity import/export authorization; and
- Power marketing liaison.

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

High Temperature Superconductivity for Electric Systems works in partnership with industry to perform the research and development required for U.S. companies to commercialize High Temperature Superconductivity (HTS) for electric power applications. To achieve commercialization of the technology, the Superconductivity Program engages in research and development which aims to 1) improve the performance of superconducting wire while reducing manufacturing costs (Wire Technology), 2) demonstrate the applicability and the potential benefits of superconductivity in electric power systems (Systems Technology) and 3) conduct the fundamental investigations necessary to support the wire and systems development (Strategic Research).

Wire research seeks methods to produce HTS wire that has higher current carrying capacity, better magnetic field capabilities, reduced manufacturing costs, and better application characteristics such as durability, flexibility, and tensile strength. Near-term research in this area focuses on conquering scale-up issues of mass-production wire technologies for coated conductor YBCO (yttrium barium copper oxide). Second generation wire development builds on the strategic research efforts to resolve fundamental barriers that limit the manufacture and applications of these exciting materials. Application of these scientific results should enable increased rates of wire fabrication along with improved properties that lower the wire and device costs for industrial partners. Longer-term wire research activities are investigating the underlying superconductivity physics.

Systems research and development activities focus on the research, development, and testing of prototype HTS power system applications through industry-led projects. Research teams investigate adaptability issues for using superconducting wire in power system applications, which include transmission cables, generators, transformers, fault-current limiters, and flywheel electricity systeMs. In addition, program efforts target end-user applications in energy-intensive industries, including large electric motors (over 5000 HP), MRI medical units, and magnetic separators. Application issues include the development of efficient cryogenic systems, cable winding techniques, and magnetic field research.

Strategic research conducts advanced, cost-shared, fundamental research activities to better understand relationships between the microstructure of HTS materials and their ability to carry large electric currents over long lengths. New projects will be added to investigate the varied technical aspects of this key problem. The benefits will be higher performance wires and inherently lower manufacturing costs. Also, work on enabling technologies such as joining HTS conductors to normal conductors will be supported as well as additional research on electrical losses due to alternating currents. These losses can be reduced through better understanding of technical parameters. This research will support new discoveries and innovations for the Second Generation Wire Development. These efforts complement research work funded by the DOE Office of Science. This subprogram includes work on planning and analysis of potential program benefits as well as communication and outreach to gather information on future requirements for the HTS technologies and to maintain contact with stakeholders.

FY 2003 saw a reorganization of the Superconductivity Program’s parent organization, from an element of the Office of Energy Efficiency and Renewable Energy’s (EERE) Distributed Energy and Electric Reliability (DEER) Program to the newly created Office of Electric Transmission and Distribution (OETD). OETD’s mission is to lead a national effort to help modernize and expand America’s electric delivery system to ensure a more reliable and robust electricity supply, as well as economic and national security.

FY 2003 also saw a very slight increase in the annual operating budget of High Temperature Superconductivity for Electric Systems from the prior year and approximately equal to the FY 2001 budget. This relatively flat funding profile has stalled new initiatives and research thrusts. The result was somewhat lower spending on capital equipment for national laboratories, as well as the postponement of the awarding of several new university projects and industry-led demonstration projects. Results that will be presented at the Peer Review in summer 2004 will determine what, if any, effect the reduction will have in achieving milestones for the long term commercialization of the technology.

DOE Contact: Jim Daley (202) 586-1165

222. **SECOND GENERATION WIRE DEVELOPMENT**
$17,330,000
National Laboratories:
Argonne National Laboratory Contact:
U. Balachandran (630) 252-4250
Brookhaven National Laboratory Contact:
David Welch (631) 344-3517
Los Alamos National Laboratory Contact:
Dean Peterson (505) 665-3030
National Renewable Energy Laboratory
Contact: Raghu Bhattacharya
(303) 384-6477
Oak Ridge National Laboratory Contact:
Robert Hawsey (615) 574-8057
Sandia National Laboratory Contact: Paul Clem
(505) 845-7544
Industry Partners:
American Superconductor Contact:
John Scudiere (508) 836-4200
SuperPower Contact: Phillip Pellegrino
(518) 346-1414
Oxford Superconducting Technology Contact:
Seung Hong (732) 541-1300
MicroCoating Technologies Contact:
Todd Polley (678) 287-2421

Second Generation Wire Development focuses on processing science and technology for fabricating HTS wire possessing all the following minimum performance characteristics: 1) length- 100-1000 m; 2) current - 100-1000 A/cm-width; 3) current density - 10^4-10^5 A/cm^2; 4) magnetic field tolerance - 2-5 T; 5) operating temperature - 20-77 K; and 6) strain tolerance - 0.2-0.3% with no degradation in current density.

Another objective is to work with U.S. industry to produce cost-effective (10-100 $/kA-m), long-length HTS wire that can support development of applications such as transformers, motors, generators, current limiters, and transmission lines. The project also will configure wires and tapes into strong field forms suitable for electric power devices.

Extending the ultimate performance of kilometer lengths of HTS wires and tapes cooled with liquid nitrogen and in magnetic fields above 2T is a central technological objective. Mature commercial production (learned-out wire cost of less than $10/kA-m) of long lengths of HTS coated conductor tapes carrying currents of 1000 amps/cm-width at current densities above 1 MA/cm^2 in magnetic fields above 2 T and 77 K should result from DOE collaborations. In the interim, development of HTS tapes based on BSCCO (bismuth strontium calcium copper oxide) will continue to be explored by DOE and its partners as a bridge to the future.

Second Generation Wire Development capitalizes on two processing breakthroughs announced in 1995 and 1996: the Ion-Beam Assisted Deposition (IBAD) process refined by LANL and the Rolling Assisted Biaxial Texturing (RABiTS) technique pioneered by ORNL. Since then, industry-led consortia have evolved to develop these techniques into viable commercial processes for making HTS wire.

Project subtasks are as follows:

Metallo-Organic Chemical Vapor Deposition (MOCVD) - Investigation continued on the development of a MOCVD technique for deposition of long-length, Yttrium-Barium-Copper Oxide (YBCO) conductors. The goal is to establish processing conditions to deposit buffer and superconducting layers on textured metallic substrates. The substrates, buffer, and superconducting layers will be characterized.

Thick HTS films - Teams made significant progress in 2003 in the development of thick HTS filMs. The films will be deposited on flexible tapes containing oxide buffer layers deposited by IBAD. Efforts continued to include analysis of electrical flow in thick films, and the development of new diagnostic techniques for identifying “bottlenecks” in the superconductors.

Substrate development - Efforts at producing long lengths of textured nickel tape with all the appropriate characteristics for subsequent film growth (buffer layer(s) and superconductor) were continued. Copper-based RABiTS type substrates were fabricated and tested with conductive and non-conductive buffer layers.

IBAD Research – Enhanced performance and reproducibility of IBAD MgO coated conductors were achieved. IBAD MgO offers significant cost benefits compared to IBAD YSZ. In 2003, improvements were made in reel-to-reel substrate electropolishing, developing a new IBAD nucleation layer (Y_2O_3), processing refinements, developing a new buffer layer ($SrRuO_3$), and improving MgO texture resulting in critical current density equal to single crystal substrates.

YBCO/RABiTS - Development and demonstration of the fabrication of lengths of YBCO/RABiTS using MOCVD technology continued. Simpler, faster, lower-cost alternate buffer layer architectures were developed that are compatible with the TFA-YBCO process. Mechanical and processing conditions needed to develop the desired surface texture and smoothness of the bare nickel were investigated. The focus is on solving problems associated with reel-to-reel continuous processing of coated conductors. In addition to providing samples of short and long-length RABiTS, program researchers continued to characterize products for uniformity of texture and electrical and mechanical properties.

Keywords: Superconductor, Coated Conductor, Buffer Layers, Deposition, Textured Substrate

223. **SYSTEMS TECHNOLOGY - PARTNERSHIPS WITH INDUSTRY**
$15,650,000

A goal of the Superconductivity Program is to develop continuous-duty, high capacity electric power equipment that has significant advantages (efficiency, size, weight) compared to equipment now in use. The Superconductivity Partnership with Industry (SPI) is an industry-led venture between the Department of Energy (DOE) and industrial consortia intended to accelerate the use of high-temperature superconductivity (HTS) in energy applications. Each SPI team includes a vertical integration of non-competing companies that represent the entire spectrum of the research and development (R&D) cycle. That is, the teams include the ultimate user of the technology (an electric power company), as well as a major manufacturing company and a supplier of superconducting components. Each team also includes one or more national laboratories that perform specific tasks defined by the team. The SPI goal is to design cost-effective HTS systems for electricity generation, delivery, and use. The funding amount includes DOE's share of the SPI design activities, as well as parallel HTS technology development that directly supports the SPI teaMs. All of these projects incorporate high-temperature superconducting wire into a utility electric application.

In FY 2003, several new projects were selected from a solicitation for industry-led, HTS power demonstration projects. However, due to lengthy negotiations and a reduced HTS budget, several programs did not get awarded until late in 2003 or early 2004.

Project subtasks are as follows:

MOTORS

The project, led by Rockwell Automation, completed operational testing of a 1,000 horsepower (hp) motor in 2001. In 2003, design studies for a 5,000 horsepower motor using HTS tape for the windings were completed. Rockwell's success with the 1,000 horsepower motor, which under load produced over 1,600 horsepower, has the company looking forward to building a larger motor with new YBCO superconducting tapes. Superconducting motors can have a large impact on electrical energy utilization through reduced losses and size compared to conventional iron core motors. These reduced losses and the smaller size will be the driving force for the commercial introduction of superconducting motors in industrial applications.

Rockwell Automation Contact: David Driscoll
(216) 266-6002

TRIAXIAL COLD DIELECTRIC SUPERCONDUCTING DISTRIBUTION CABLE

Ultera (a partnership between Southwire Company and NKT) and DOE completed an agreement to enter a new phase of a partnership centered on the development of a power cable for real-world applications. Ultera began work, in conjunction with Oak Ridge National Laboratory, on a new triaxial design for a 100-meter, three phase (13.2 kV, 3 kA, 69 MVA) power cable to be installed at a substation in Columbus, Ohio. The project builds on an earlier SPI success, the 30-meter, 27 MVA, three-phase HTS cable that was completed in 2000 and feeds electricity to three Southwire manufacturing facilities.

Ultera Contact: David Lindsay (770) 832-4916

COLD DIELECTRIC SUPERCONDUCTING DISTRIBUTION CABLE (WITH YBCO SEGMENT)

SuperPower and utility host, Niagara Mohawk, were awarded this new HTS cable project to demonstrate a 350-m underground HTS distribution (34.5 kV, 800 A, 48 MVA) cable in the utility grid. The initial cable will use BCCCO conductors. A 30-m BSCCO cable segment would later be replaced and tested with a second generation YBCO cable segment.

SuperPower Contact: Philip Pellegrino (518) 346-1414

COAXIAL COLD DIELECTRIC SUPERCONDUCTING TRANSMISSION CABLE

American Superconductor, with Long Island Power Authority (LIPA), Nexans, and Air Liquide, were awarded this new HTS cable project to demonstrate a 610-m transmission (138 kV, 2.4 kA, 600 MVA) cable that would provide 2-5 times the power transfer capacity within the existing rights-of-way to meet the expected load growth in Long Island. This will be the world's first transmission voltage HTS cable.

American Superconductor Contact: Michael McCarthy (508) 621-4380

WARM DIELECTRIC SUPERCONDUCTING TRANSMISSION CABLE

This HTS cable project (24 kV, 2.4 kA, 100 MVA) was completed and decommissioned in 2003 after successfully testing one phase of the cable. The project had to overcome problems with vacuum leaks in the cable. The team was led by Pirelli Cables and Systems and included Detroit Edison, American Superconductor, and Los Alamos National Lab. The HTS cable will lead to smaller, more efficient electricity transmission lines in utility networks.

Pirelli Contact: Nathan Kelley (803) 356-7762

FLYWHEEL ELECTRICITY SYSTEM

FY 2003 saw the successful demonstration of a 10 kWh Flywheel Electricity System designed and built by a team led by Boeing. High Temperature Superconducting bearings, made from a bulk superconductor material, are an enabling technology for the flywheel design. The bearings allow the flywheel to store electricity with increased efficiency. A follow-on project was awarded for the demonstration of a 35 kWh power risk management system using the flywheel and superconducting bearings.

Boeing Contact: Mike Strasik (425) 237-7176

RECIPROCATING MAGNETIC SEPARATOR

This project teams DuPont with the National High-Magnetic Field Laboratory to develop a reciprocating magnetic separator. These devices are used in the materials field and are traditionally large consumers of utility electricity. In 2001, a ¼ scale demonstration unit was assembled and tested. The unit exceeded expectations, and in 2002 DuPont reached an agreement with DOE to build and test a full-scale, pre-production Reciprocating Magnetic Separator.

DuPont Contact: Chris Rey (302) 695-9470

TRANSFORMER

Waukesha Electric Systems (WES) is leading a team that includes ORNL, IGC-SuperPower, and Rochester Gas and Electric to build and operate a 5/10 MVA alpha prototype cryocooled HTS power transformer on the Wisconsin Electric Power utility grid. The prototype will power WES' main transformer manufacturing plant. In 2003, the team completed the assembly and testing of the transformer. Some high-voltage problems have surfaced, and Waukesha and ORNL have solved these probleMs. The unit is ready for operational testing on the grid.

ORNL Contact: Bob Hawsey (865) 574-8057

MRI

Oxford Superconducting Technology began a project in 2002 to demonstrate a cost-effective, open-geometry MRI (magnetic resonance imaging) system. MRIs represent the greatest existing market for low temperature superconductors, and use tremendous amounts of electricity to create their powerful magnetic fields. HTS technology has the potential to allow for smaller, more flexible MRI designs, as well as huge reductions in the amount of electricity and utility infrastructures required to operate the devices. Oxford has completed several proof-of-concept devices, but the new project will involve establishing a continuous melt process for dip-coated BSCCO 2212 superconducting tape.

Oxford Contact: Kenneth Marken (732) 541-1300

GENERATOR

General Electric Corporate Research and Development is leading a team that includes ORNL, American Electric Power, and PG&E to develop and demonstrate a 100 MVA HTS generator. HTS generators will have improved efficiency, higher capacity, and improved reactive power capabilities. The project was awarded in 2002, and GE has completed conceptual designs and began component acquisition/fabrication.

ORNL Contact: Bob Hawsey (865) 574-8057

CURRENT LIMITER

SuperPower, in partnership with Nexans, ORNL, LANL, ANL, and EPRI, began a new project to demonstrate an HTS fault current limiter at 138 kV (transmission level voltages) using existing melt-cast processed BSCCO-2212 bulk conductors. Current limiters can be used on transmission and distribution systems to protect system components from damaging power surges caused by ground faults. Compared to conventional devices, HTS current limiters offer better protection and improved system flexibility, reliability, and performance without active controls or power electronics and without multiple circuit breaker upgrades.

SuperPower Contact: Philip Pellegrino (518) 346-1414

Keywords: Motor, Generator, Magnetic Resonance, Current Limiter, Transmission Cable, Flywheel, Separator

224. **STRATEGIC RESEARCH**
$5,030,000
Argonne National Laboratory Contact:
U. Balachandran (630) 252-4250
Brookhaven National Laboratory Contact:
David Welch (516) 282-3517
Los Alamos National Laboratory Contact:
Dean Peterson (505) 665-3030
National Renewable Energy Laboratory Contact:
Raghu Bhattacharya (303) 384-6477
Oak Ridge National Laboratory Contact:
Robert Hawsey (615) 574-8057
Oxford Superconducting Technology Contact:
Seung Hong (732) 541-1300
University of Wisconsin Contact:
David C. Larbalestier (608) 263-2194

Strategic research and development projects in the program are crucial for the discovery of new technologies, such as RABiTS and magneto-optical imaging (MOI) that make the program a world leader in the race to bring HTS electric power technologies to market. Critical theoretical calculations, new material evaluation, and process development support the program's industry-directed Cooperative Research and Development Agreement (CRADA) work and the SPI application projects and provide a foundation for future collaborations and progress toward HTS commercialization by industry.

Work by all organizations in strategic research comprises a diverse set of topics from characterization techniques to wire processing to applications development. As these activities mature, they evolve into more cohesive efforts devoted to improving mechanical and electrical properties of wire and new devices.

Project subtasks are as follows:

Strategic projects continued to focus on the development of improved substrates for both IBAD and RABiTS processes, and deposition processes for buffer layers and the superconductor layer. Characterization of buffer and superconductor layers attempted to correlate processing parameters with final wire performance. Projects were active at all six national laboratories.

Wire Characterization - Program participants were continuing the characterization of microstructural and superconducting properties of second-generation wire to improve understanding of J_c-limiting factors related to the formation and growth kinetics of high-temperature superconductors. On-line characterization instruments are being developed to maintain quality control in the fabrication of long lengths of HTS wire. The engineering scale-up will require the integration of characterization and the process control of the fabrication parameters.

Oxide buffer layer research - Work on developing sol-gel derived oxide buffer layer systems continued in 2003. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties. Additionally, Sandia scientists worked on developing high-quality, solution-derived, 123-type superconducting films for coated conductor applications.

Coated conductor processing - Research and development of YBCO coated conductor processing continued in a variety of subtasks. Scale-up issues are being defined and addressed. Developing the capability to fabricate long lengths on RABiTS, using electron beam evaporation and an existing ultra-high vacuum, reel-to-reel system remained a priority. Lengths of RABiTS were being provided for internal use as well as for various partners.

PLD Deposition - A system and process for deposition of YBCO by Pulse Laser Deposition on moving substrates was being developed by the utilization of a radiant heating system, along with sample translation. Also, improved texture in substrates with reduced magnetism was under development. New RABiTS architectures, with conductive and simpler structures, were investigated.

Process technology - DOE partners worked toward developing and demonstrating process technology needed for epitaxial growth of buffer layers by metalorganic decomposition. A specific objective of the project is to develop alkoxide precursor methods for deposition of buffer layers compatible with textured metallic substrates appropriate to long-length conductor manufacture and compatible with American Superconductor's YBCO deposition methods.

The program supports a broad range of activities which concentrate on the underlying principles of HTS and developing an understanding of how these principles affect final HTS material properties. Collaborators in the activities have worked on understanding reaction kinetics, effects of stoichiometry on the superconducting properties, introducing flux pinning centers, and monitoring current transport in HTS conductors.

AC loss characterization - Attempts to characterize AC losses in HTS tapes, under conditions which simulate the electromagnetic conditions in utility devices, continued. Program participants worked to design a cable configured to minimize AC losses.

Keywords: Superconducting Tapes, Flux Pinning, Bismuth Conductor

OFFICE OF SCIENCE

	FY 2003
OFFICE OF SCIENCE - GRAND TOTAL	$607,694,828
OFFICE OF BASIC ENERGY SCIENCES	$550,604,000
DIVISION OF MATERIALS SCIENCES AND ENGINEERING	$233,940,000
Theoretical Condensed Matter Physics	16,993,000
Experimental Condensed Matter Physics	37,205,000
Materials Chemistry	40,563,000
Mechanical Behavior and Radiation Effects	13,323,000
X-ray and Neutron Scattering	37,821,000
Structure and Composition of Materials	28,915,000
Physical Behavior	20,262,000
Synthesis and Processing Sciences	11,839,000
Engineering Physics	15,297,000
Experimental Program to Stimulate Competitive Research	11,722,000
DIVISION OF SCIENTIFIC USER FACILITIES	$316,664,000
X-ray and Neutron Scattering Facilities	281,013,000
Nanoscience Centers	35,651,000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH	$45,870,828
TECHNOLOGY RESEARCH DIVISION	$45,870,828
LABORATORY TECHNOLOGY RESEARCH PROGRAM	$749,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING	$528,000
Advanced Processing Techniques for Tailored Nanostructures in Rare-Earth Permanent Magnets (Al 01 02)	241,000
Low-cost, High-performance YBCO Conductors (ORNL 01 06)	287,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR, OR TESTING	$221,000
Nanofabrication of Advanced Diamond Tools (LBNL 01 03)	221,000
SMALL BUSINESS INNOVATION RESEARCH PROGRAM	$42,060,212
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$12,898,381
FY 2003 PHASE I	$3,595,018
Solid State SPECT Detectors for Molecular Imaging in Small Animals	100,000
Fast, High Resolution Pet Detector	100,000
A Remote and Affordable Detection System for Cr(VI) in Groundwater	99,998
Nanoscale Inorganic Ion-Exchange Films for Enhanced Electrochemical Heavy Metal Detection	99,999
SiC/HT-9 MMC Composite Tubes for Fuel Cladding	100,000
Improved Silicon Carbide Materials for Very High-Temperature, Fast-Spectrum Nuclear Energy Systems	99,805

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
FY 2003 PHASE I (continued)	
A GEM of a Neutron Detector	99,988
Amorphous, Silicon-Based Neutron Detector	100,000
Long-Lifetime, Low-Scatter Neutron Polarization Target	99,985
Polymer White Light Emitting Devices	99,800
Novel Light Extraction Enhancements for OLED Lighting	100,000
Molecular-Sieve-Based Nano-Cathode Structures for PEM Fuel Cells	100,000
Enhanced Optical Efficiency Package Incorporating Nanotechnology Based Downconverter and High Refractive Index Encapsulant for AlInGaN High-Flux White Led Lamp with High Luminous Efficiency	99,838
Efficient Hybrid Phosphors for Blue Solid State Light Emitting Diodes	99,984
Novel, Low - Cost Technology for Solid State Lighting	99,976
Fiber Optic Hydrogen Sensors Based on Nano-sized Metal Alloys	99,767
Universal Photo-Acoustic Sensor System	99,993
Contamination-Resistant Two-Phase Membranes for High-Temperature Hydrogen Separation	100,000
Real-Time In-Situ Monitoring of Combustion Gas Mixtures by Microporous Solid Array Sensor	98,400
Advanced Thermal Spray Fabrication of Solid Oxide Fuel Cells	98,931
Low Cost Spray Deposition for SOFC Manufacturing	100,000
Low-Cost Rapid Joining for Fabrication/In-Situ Repair of Large SiC Composite Structural Materials for Fusion Reactors and Other Commercial Applications	100,000
Low-Cost Fabrication of Inertial Fusion Energy Capsule Supports	99,766
Microengineered Tungsten Firstwall Structure for Inertial Fusion Energy Reactors	99,999
Design and Testing of a Fast-Release Tilted Target for RIA	99,079
Microchannel Plate Hard X-Ray Imaging Detector	100,000
New N+ Contact for Germanium Strip Detectors	100,000
Ball Grid Array Compatible, Optical Packaging and Assembly Process	99,994
Geiger Photodiode Array Readouts for Scintillating Fiber Arrays	99,812
Joining of Ceramic Structures for Advanced High Energy Accelerators	100,000
Extrusion of Tin Hole in Subelements for Internal-Tin Nb_3Sn Superconductor	100,000
A High Current Density, Low Magnetization, Tubular Filamented Nb_3Sn Superconductor	99,906
Development of Internal-Tin Nb/Sn Strand for High Field Accelerator Dipole Applications	100,000
Engineered Ceramic Composite Insulators for High Field Magnet Applications	99,998
An Internal Tin Tube Process for High Performance Nb_3Sn Conductors	100,000
Thermo-Magnetic Continuous Processing of Bi-2212 Cable for HEP	100,000
FY 2003 PHASE II (FIRST YEAR)	$4,492,399
Perovskite/Oxide Composites as Mixed Protonic/Electronic Conductors for Hydrogen Recovery in IGCC Systems	374,909
Highly Textured Composite Seals for SOFC Applications	375,000
Biomimetic Membrane for Carbon Dioxide Capture from Flue Gas	369,372
Low-Cost Nanoporous Sol Gel Separators for Lithium-Based Batteries	288,552
New Solid State Lighting Materials	374,907
Transformer Ratio Enhancement Experiment for Next Generation Dielectric Wakefield Accelerators	300,000

OFFICE OF SCIENCE

		FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)		
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING(continued)		
FY 2003 PHASE II (FIRST YEAR) (continued)		
High Current Density (Jc), Low AC Loss, Low Cost Internal-Tin Superconductors		374,911
Microwave Component Fabrication using the Fast Combustion Driven Compaction Process		374,835
Micro-Photomultiplier Array		360,370
Electrically Medicated Microetching Manufacturing Process to Replace Emersion and Spray Etching		374,960
Separation and Enrichment of Xenon in Air		299,939
High Performance Thermo-Electrically-Cooled LWIR Mercury Cadmium Telluride Detectors		250,000
VEGF-Based Delivery of Boron Therapeutics		374,644
FY 2003 PHASE II (SECOND YEAR)		$4,810,964
A High-Power, Ceramic, RF Generator and Extractor		375,000
KA-Band RF Transmission Line Components for a High-Gradient Linear Accelerator		375,000
A Method to Increase Current Density in a Mono Element Internal Tin Process Superconductor Utilizing ZrO_2 to Refine the Grain Size		374,988
Hermetic Metallization of Aluminum Nitride for Radio Frequency Devices		374,993
A Liquid-Desiccant Heating/Cooling System Powered by Solar Energy		374,482
Truss-Integrated Thermoformed Ductwork		375,000
Novel Membrane Reactor for the Desulfurization of Transportation Fuels		375,000
Low Emission Diesel Engines		375,000
Low-Cost, Large-Membrane-Area Modules for Gas Separation		311,764
Novel Nano-Structured Catalyst for Steam Gasification of Carbonaceous Feedstocks		375,000
Amended Silicate Sorbents for Mercury Removal from Flue Gas		375,000
Control of Catalyst Poisons from Coal Gasifiers		375,000
High-Temperature Highly-Efficient Ceramic Heat Exchanger		374,737
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING		$6,683,608
FY 2003 PHASE I		$3,263,957
A Design of a New Readout Sensor for Spect		100,000
High Performance Pet Detector		100,000
Enhanced Materials for Reactive Barriers		100,000
Novel Permeable Reactive Barrier Materials for the Mercury Plume		98,830
Electrodecontamination for Mitigation of Airborne Contamination		100,000
Improved Method to Convert Coal to Liquid Fuels		98,315
Characterization of Solid Oxide Fuel Cell Components Using Electromagnetic Model-Based Sensors		99,878
Harsh-Environment, Fiber-Optic Sensing System for SOFC Applications		97,932
A Novel Process for the Application and Finishing of Nanocrystalline Superhard Steel onto Internal Combustion Engine Components		99,925
Evaluation of a Novel Magnetic Activated Carbon Process for Gold Recovery		92,623
Tailorable, Environmental Barrier Coatings for Super- Alloy Turbine Components in Syngas		99,661
Hot Section Material Systems Testing and Development for Advanced Power Systems		89,717
Advanced Thermal Barrier Coatings for Turbine Components		99,992
SiCN High Temperature Microelectromechanical Systems (MEMS) Sensor Suite		99,878

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
FY 2003 PHASE I (continued)	
Enhanced Performance Carbon Foam Heat Exchanger for Power Plant Cooling	99,687
Selective Adsorption Membranes for Natural Gas Upgrading	99,473
Dehydration of Natural Gas	100,000
Membranes for Methane/Nitrogen Seperation	100,000
High Pressure Economical Process for Treating Natural Gas	100,000
A Novel Oxidation Process for the Conversion of Coal to Diesel Fuel-Grade Chemicals	100,000
Novel Fischer-Tropsch Reactor	100,000
Innovative Inorganic Fusion Magnet Insulation Systems	99,100
Vacuum Pressure Impregnation Insulation Systems for High Temperature Fusion Applications	98,802
Thermomechanical Processing of Nb for Improved Superconductor Applications	99,280
Preceramic Precursor Routes to Tailorable, Low-Activation, Silicon-Carbide-Based Joints	99,378
An Advanced Monolithic NbTi Conductor with 5 Tesla Jc of 5000 A/mm^2 and Beyond for Use in Superconducting Quadrupole Magnets	100,000
Aluminum Nitride Radio Frequency Windows	92,014
A New SRF Cavity Processing Technique for the Elimination of Field Emission and Surface Preparation in Fully Assembled Cavities	100,000
A Novel Design for CZT Gamma Ray Spectrometers	100,000
Compact Surface Mount Miniature Photomultipliers	99,569
Some Improved Methods of Introducing Additional Elements into Internal-tin Nb_3Sn	99,989
Fast X-Band Phase Shifter	100,000
Near Net Shape Manufacturing Using Combustion Driven Compaction	99,914
FY 2003 PHASE II (FIRST YEAR)	$749,974
Multilayer Composite Membranes for Upgrading Acid-Rich Natural Gas	375,000
Stabilized Lithium Manganese Oxide Spinel Cathode for High Power Li-Ion Batteries	374,974
FY 2003 PHASE II (SECOND YEAR)	$2,669,677
Doppler Laser Radar for Non-Intrusive Liquid Metal Flow Characterization	371,942
Multi-Megawatt Circulator for TE01 Waveguide	125,000
Active Vibration Control of NLC Magnets	375,000
An Electrical Condition Monitoring Approach for Wire and Cable	300,000
X-Ray Diagnostics for High-Temperature Superconductor Processing	375,000
Non-Invasive Techniques to Study Local Passivity Breakdown of Metal Alloys in Aqueous Media	372,896
Microelectrode Array for Electrochemical Sensing of Localized Corrosion	374,839
Intelligent Probes for Enhanced Non-Destructive Determination of Degradation in Hot-Gas-Path Components	375,000
Al(In)GaN-Based, High-Electron Mobility Transistors (HEMTs) on SiC for High-Power Radar Applications	99,997
Cell-Free Protein Synthesis for High-Through-Put Proteomics	100,000
A New Class of Trimetasphere Based Radiopharmaceuticals	97,636
Low-Cost Automatic Tool Fixturing Based on Dexterous Robotic Hand	100,000
Nanoengineered ODS Feritic/Martensitic Steel for Fusion Application	99,983
Low-Porosity SiC/SiC Composite Materials for Nuclear Energy System Components	99,993

	FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$15,421,619
FY 2003 PHASE I	$4,284,392
Solid-State Thermal-Neutron Detector Based on Boron-Doped a-Se Stabilized Alloy Films	100,000
New, Stable Cathode Materials for OLEDs	99,780
Novel Lower-Voltage OLEDs for Higher-Efficiency Lighting	100,000
Nanowire Cathode Material for Lithium-Ion Batteries	99,676
High Performance Solid Polymer Electrolyte for Lithium Batteries	100,000
Multi-Layer Anode Stabilization Layer For Preventing Dendrites and Li Corrosion In Lithium-Sulfur Batteries	96,908
Highly Conductive Solvent-Free Polymer Electrolytes for Lithium Rechargeable Batteries	100,000
$LiFePO_4$ Cathode Material Designed for Use in Lithium-Ion Batteries with Application to Electric and Hybrid-Electric Vehicles	98,064
Preparation of High Performance Nanocomposite Cathode Materials	99,995
High Energy Density Rechargeable Lithium Sulfur Battery with Novel Solid Electrolyte	100,000
Polysiloxane-Transition Metal Complex Copolymer Catalysts for Asymmetric Transformations	99,995
Metal Oxide Catalyst for Methyl Ethyl Ketone Production via One-Step Oxidation of n-Butane	99,996
Discovery and Optimization of New Heterogeneous Catalysts for the Direct Production of Propylene Oxide (PO) from Propylene and Oxygen Using Combinatorial Methods	99,999
Nano-Zeolite Coatings on Microlith Substrates for High Selectivity Chemical Reactions	100,000
Novel Catalytic Technology for Propylene Epoxidation	100,000
New Nanostructured Polymeric Membrane for Direct Methanol Fuel Cells	100,000
Low Cost and High Performance, Polymer Nanocomposite, Specialty Industrial Coatings	100,000
PET Nanocomposites for Beverage Container Applications	100,000
Ultra-Hard Nanostructured Silicon Carbide for Deep-Hole Drilling	99,982
Industrial Nano Material Components with High Temperature Corrosion and Wear Resistance Performance for Energy Savings	100,000
A New Composite Proton Exchange Membrane	95,756
CCVD-Produced, Oxygen-Deficient, Nanocrystalline Perovskite for Low-Temperature Proton Exchange Membranes	100,000
High Temperature-Stable Membrane Electrode Assemblies for Fuel Cells Fabricated via Ink Jet Deposition	99,999
Membrane Separation Combined with Catalytic Biomass Gasification to Produce Hydrogen-Rich Gas	99,787
UV LEDs for Solid State Lighting	99,694
Efficient Incandescent Visible Light Produced by Improved Boride and Nitride Filament Radiation	99,966
Gallium-Nitride Substrates for Improved, Solid-State Lighting	100,000
An Optical Fiber Probe for the Measurement of High Temperatures	97,500
Cost Effective Improved Refractory Materials for Gasification Systems	99,964
Dense Membrane for Hydrogen Separation Based on High Proton Conductivity and Chemical Stability	100,000
Development of Protective Coatings for Single-Crystal Turbine Blades	99,881
Advanced Net-Shape Insulation for Solid Oxide Fuel Cells	99,848
High-Performance, Plasticization-Resistant Membranes for Natural Gas Separations	100,000
Cost Effective Fischer-Tropsch Technology	100,000
Nanocomposite Dielectric Materials for High Frequency Applications	99,995
Combinatorial Strategy Toward Fast and Efficient Scintillators	99,998
Very Large, High Gain APDs for Particle Physics	100,000

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
FY 2003 PHASE II (FIRST YEAR)	$5,574,794
Embedded Sensors in Turbine Systems by Direct Write Thermal Spray Technology	349,881
Catalyst to Improve Small-Scale Claus Plants	375,000
LSGM Based Composite Cathodes for Anode Supported, Intermediate Temperature (600-800 degrees C) Solid Oxide Fuel Cells (SOFC)	249,634
Metal Oxide Catalyst for Methacrylic Acid Preparation via One-Step Oxidation of Isobutane	374,998
P-Type ZnO Films	375,000
An Advanced Cathode Material for Li-Ion Battteries	374,580
Three-Dimension Woven Carbon-Glass Hybrid Wind Turbine Blades	333,188
Feasibility of Cost Effective, Long Length, BSCCO 2212 Round Wires, for Very High Field Magnets, Beyond 12 Tesla at 4.2 Kelvin	311,806
Growth of a New, Fast Scintillator Crystal for Nuclear Experiments	374,423
A New Scintillator for Gamma Ray Spectroscopy	375,000
Diamond Windows for High Power Microwave Transmission	373,149
Radiation Resistant Insulation with Improved Shear Strength for Fusion Magnets	374,707
Nanostructured Tungsten for Improved Plasma Facing Component Performance	375,000
Low Cost Materials for Neutron Absorption in Generation IV Nuclear Power Systems	299,750
High Resolution Gamma Ray Spectrometer for Nuclear Non-Proliferation	375,000
Growth of a New Mid-IR Laser Crystal	374,709
Induim Arsenide Antimonide Very Long Wavelength Photodiodes for Near Room Temperature Operation	246,199
FY 2003 PHASE II (SECOND YEAR)	$5,562,433
Innovative Organic and Inorganic High-Pressure Laminate Insulation for Fusion and Superconducting Magnets	373,651
Inorganic-Organic Hybrid Materials: Diacetylene-Siloxanes as Radiation Resistant Electrical Insulator for Plasma Fusion Confinement Systems	374,999
Ultra-Thin Optical Diagnostic Filters for Plasma Wakefield Accelerators	340,034
Enhanced Efficiency Nanowire Photocathode for Large PMTs	375,000
Superinsulation for Ductwork	375,000
Recycling of Coated Plastics Used in Automotive, IT and Commercial Applications	349,333
Two-Step Methane Conversion to Alkynes and Dienes	375,000
Improved Buffered Substrates for YBCO Coated Conductors	375,000
Low Cost Carbon Micro Bead Anodes for Lithium-Ion Batteries	375,000
A Novel Cathode Material for High Power Lithium Rechargeable Batteries	375,000
Development of Low-Cost Salts for Lithium-Ion, Rechargeable Batteries	374,850
High-Performance Carbon Materials for Ultracapacitors	374,888
Synthesis of Bulk Amounts of Double-Walled Carbon Nanotubes	375,000
Intermediate Temperature Solid Oxide Fuel Cell Development	374,678
Novel Ceria-Based Materials for Low-Temperature Solid Oxide Fuel Cells	375,000

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES	$6,610,433
FY 2003 PHASE I	$3,743,216
Situational Awareness Monitor for Nuclear Events	100,000
Low-Noise Borehole Triaxial Seismometer	99,961
Compact, Short-Pulse Laser Source for Active Imaging Systems	99,297
Advanced, Aerosol Mass Spectrometer for Aircraft Measurement of Organic Particulate Matter	100,000
Cavity Attenuation Phase Shift Spectroscopic Detection of Nitrogen Dioxide	100,000
Novel Ultrasensitive Instrumentation for Trace Gas Measurements in the Field	99,999
NO_2 Sensor for Urban and Regional Air Quality Monitoring	99,994
Fiber-Laser-Based Water Vapor Differential Absorption Lidar System	91,058
Innovative Carbon Dioxide Sensor Based on Cavity Ringdown	99,958
High Precision CO_2 Sensor for Balloon Sonde Atmospheric Measurements	100,000
Innovative Instrumentation and Intelligent Diagnostic System for Reactor Safety	100,000
Real-Time Monitoring of Catalytic Surfaces for Petrochemical Synthesis Using a Mass-Heat Flow Sensor	100,000
A Down-Hole Probe for Real-Time Ore Grade Assessment in “Look Ahead” Mining	99,909
Development of HSTAT for HVAC Health Status and Control	99,986
First-Ever Mobile System for In Situ Acquisition of Isotope Data on Natural Gas	84,719
Low-Cost Distributed Sensing for Gas Pipelines	99,966
A Reliable Optical System for Natural Gas Pipeline Leak Detection	100,000
Downhole Spectrometric Device for the Real-Time Analysis of Fluid Composition	99,702
An Extremely High Power, Field-Coupled, Low-Loss RF Transmission Line for SRF Cavities	100,000
Magnetized Electron Transport in the Proposed Electron Cooling Section of the Relativistic Heavy Ion Collider	99,970
Ultra High Speed Analog to Digital Converter with Ternary Digital Output	99,758
Pulse-Synchronized Serializer/De-Serializer-Based Interconnect	99,994
New Hybrid Pulse-Processor for X- and Gamma-Ray Spectroscopy	100,000
Digital Signal Processing for Nuclear Physics Applications	81,926
High-Speed Centralized Intrusion Detection Device	99,994
High Speed Optical Source for High Energy Physics Data Acquisition	99,983
High Precision, Integrated Beam Position and Emittance Monitor	100,000
Six-Dimensional Beam Cooling in a Gas Absorber	100,000
Electron Bunch Length Diagnostic Device	100,000
High-Power Radio Frequency Window	95,525
Sheet Beam Klystron for Accelerators	100,000
Hybrid Modulator Upgrade	99,455

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES (continued)	
FY 2003 PHASE I (continued)	
NLC Marx Bank Modulator	99,767
Quasi-Optical 34-GH_z Radio Frequency (RF) Pulse Compressor	100,000
KA-Band Resonant Ring for High-Power Testing of Accelerator Components	100,000
A Hydrostatic Processing Facility for Superconducting Wire	99,495
Novel Magnetometer for Quadrupole and Dipole Magnetic Measurements	99,954
Development of Sub-Picosecond Phase Stability Signal Multipliers	92,846
FY 2003 PHASE II (FIRST YEAR)	$1,369,103
An Inexpensive, Efficient Neutron Monochromator	375,000
High Gain, Fast Scan, Broad Spectrum, Parallel Beam Wavelength Dispersive X-Ray Spectrometer for SEM	273,093
Advanced X-Ray Detectors for Transmission Electron Microscopy	375,000
Using Convergent Beams for Small-Sample, Time-of-Flight Neutron Diffraction	346,010
FY 2003 PHASE II (SECOND YEAR)	$1,498,114
Sol-Gel Derived Neutron Detector Using a Lithiated Glass	373,920
Development of an Ultra-Bright Electron Source for Scanning Transmission Electron Microscopy	375,000
Pixel-Cell Neutron Detector and Read-Out System Meeting Requirements of Present and Future Neutron Scattering Facilities	374,442
Novel Neutron Detector for High Rate Imaging Applications	374,752
MATERIALS STRUCTURE AND COMPOSITION	$446,171
FY 2003 PHASE II (FIRST YEAR)	$446,171
Development of a New, Low Frequency, Rf-Focused Linac Structure	446,171
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM	$3,061,616
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$774,988
FY 2003 Phase I	$100,000
Engineered Tungsten Surfaces for IFE Dry Chamber Walls	100,000
FY 2003 PHASE II (FIRST YEAR)	$424,988
Carbon Fiber Composite Aeroelastically Tailored Rotor Blades for Utility-Scale Wind Turbines	424,988

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
FY 2003 PHASE II (SECOND YEAR)	$250,000
Advanced Membrane Technology for Biosolvents	250,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$600,000
FY 2003 PHASE I	$100,000
Improved Electron Yield and Spin-Polarization from III-V Photocathodes via Bias Enhanced Carrier Drift	100,000
FY 2003 PHASE II (FIRST YEAR)	$250,000
Hydroforming of Light Weight Components from Aluminum and Magnesium Sheet and Tube	250,000
FY 2003 PHASE II (SECOND YEAR)	$250,000
Neutron Scattering Instrumentation for Measurement of Melt Structure	250,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,586,673
FY 2003 PHASE I	$399,998
Novel Polymer Nanocomposite Processing	100,000
Nanostructured Polymeric Heterogeneous Catalyst for Industrial Applications	100,000
Development of Silicon Nanocrystals as High Energy White Phosphors	100,000
Novel Approach Toward High Performance Energetic Rays Detection	99,998
FY 2003 PHASE II (FIRST YEAR)	$300,000
Waveshifters and Scintillators for Ionizing Radiation Detection	300,000
FY 2003 PHASE II (SECOND YEAR)	$886,675
Virtual-Impact Particle Sizing for Precursor Powders of Nb_3Sn and Bi-2212 Superconductors	164,032
Innovative Processing Methods for Superconducting Materials	227,322
Oxide Dispersed Nanofluids for Next Generation Heat Transfer Fluids	250,000
Plasma Spraying of $Nd_2Fe_{12}B$ Permanent Magnet Materials	245,321

OFFICE OF SCIENCE

	FY 2003
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES	$99,955
FY 2003 PHASE I	$99,955
Using Electrical Resistivity Techniques to Monitor the Long-Term Health of Sub-Surface Reactive Barriers	99,955
OFFICE OF FUSION ENERGY SCIENCES	$9,000,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$9,000,000
Vanadium Alloy and Insulating Coating Research	1,500,000
Theory and Modeling	1,700,000
Ferritic/martensitic Steel Research	2,300,000
SiC/SiC Composites Research	1,500,000
Plasma Facing Materials Research	2,000,000
OFFICE OF BIOLOGICAL & ENVIRONMENTAL RESEARCH	$2,220,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,220,000
Radiation Effects on Sorption and Mobilization of Radionuclides During Transport Through the Geosphere	60,000
Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes	79,000
Radiation Effects in Nuclear Waste Materials	206,000
New Metal Niobate and Silicotitanate Ion Exchangers: Development and Characterization	310,000
Physical, Chemical and Structural Evolutioon of Zeolite-Containing Waste Forms Produced from Metakaolinite and Calcined HLW	240,000
Investigating Ultrasonic Diffraction Grating Spectroscopy and Reflection Techniques for Characterizing Slurry Properties	235,000
Chemistry of Actinides in Molten Glasses and its Correlation to Structural Performance of Solid Glasses: Filling the Knowledge Gap	100,000
Stability of High Level Radioactive Waste Forms	190,000
Physical Characterization of Solid-Liquid Slurries at High Weight Fractions Utilizing Optical and Ultrasonic Methods	240,000
Assessing the State and Distribution of Radionuclide Contamination in Concrete: An Experimental and Modeling Study of the Dynamics of Contamination	300,000
Underground Corrosion After 32 Years: A Study of Fate and Transport	260,000

OFFICE OF SCIENCE

The Office of Science (SC) advances the science and technology foundation for the Department and the Nation to achieve efficiency in energy use, diverse and reliable energy sources, a productive and competitive economy, improved health and environmental quality, and a fundamental understanding of matter and energy. The Director of Science is responsible for six major outlay programs: Basic Energy Sciences, Fusion Energy, Health and Environmental Research, High Energy and Nuclear Physics and Computational and Technology Research. The Director also advises the Secretary on DOE physical research programs, university-based education and training activities, grants, and other forms of financial assistance.

The Office of Science mainly conducts materials research in the following offices and divisions:

- Office of Basic Energy Sciences - Division of Materials Sciences and Engineering
- Office of Basic Energy Sciences - Division of Scientific User Facilities
- Office of Advanced Scientific Computing Research - Division of Technology Research
- Office of Biological and Environmental Research - Medical Sciences Division
- Office of Fusion Energy - Division of Advanced Physics and Technology

Materials research is carried out through the DOE national laboratories, other federal laboratories, and grants to universities and industry.

OFFICE OF BASIC ENERGY SCIENCES

The Office of Basic Energy Sciences (BES) supports basic research in the natural sciences leading to new and improved energy technologies and to understanding and mitigating the environmental impacts of energy technologies. The BES program is one of the Nation's foremost sponsors of fundamental research in broad areas of materials sciences, chemical sciences, geosciences, biosciences, and engineering sciences. The BES program underpins the DOE missions in energy and the environment, advances energy-related basic science on a broad front, and provides unique national user facilities for the scientific community. The program supports two distinct but interrelated activities: 1) research operations, primarily at U.S. universities and 11 DOE national laboratories and 2) user-facility operations, design, and construction. Encompassing more than 2,400 researchers in 200 institutions and 17 of the Nation's premier user facilities, the program involves extensive interactions at the interagency, national, and international levels. All research activities supported by BES undergo rigorous peer evaluation through competitive grant proposals, program reviews, and advisory panels. The challenge of the BES program is to simultaneously achieve excellence in basic research with high relevance to the Nation's energy future, while providing strong stewardship of the Nation's research performers and the institutions that house them to ensure stable, essential research communities and premier national user facilities.

DIVISION OF MATERIALS SCIENCES AND ENGINEERING

The Division of Materials Sciences conducts a broad program of materials research to increase the understanding of phenomena and properties important to materials behavior that will contribute to meeting the needs of present and future energy technologies. The Division supports fundamental research in materials at DOE national laboratories and plans, constructs, and operates national scientific user facilities needed for materials research. In addition, the Division funds over 230 grants, mostly with universities, on a wide range of topics in materials research. Fundamental materials research is carried out at eleven DOE laboratories: Ames Laboratory at Iowa State University, Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Environmental and Engineering Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories in New Mexico and California, and the Stanford Synchrotron Radiation Laboratory. The laboratories also conduct significant research activities for other DOE programs such as Energy Efficiency, Fossil Energy, Nuclear Energy, Environmental Management and Defense PrograMs. The Division of Materials Sciences and Engineering also funds the University of Illinois Frederick Seitz Materials Research Laboratory. Summaries of the laboratory portion of the program and an interim listing of FY 2003 grants are available on the World Wide Web at the following address:

http://www.science.doe.gov/bes/dms/Research_Programs/research_program.htm.

The performance parameters, economics, environmental acceptability and safety of all energy generation, conversion, transmission, and conservation technologies are limited by the discovery and optimization of the behavior and performance of materials in these energy technologies. Fundamental materials research seeks to understand the synergistic relationship between the synthesis, processing, structure, properties, behavior, performance of materials of importance to energy technology applications and recycling of materials. Such understanding is necessary in order to develop the cost effective capability to discover technologically and economically desirable new materials and cost competitive and environmentally acceptable methods for their synthesis, processing, fabrication, quality manufacture and recycling. The materials program supports strategically relevant basic scientific research that is necessary to discover new materials and processes and to eventually find optimal synthesis, processing, fabricating, and manufacturing parameters for materials. Materials Science research enables sustainable development so that economic growth can be achieved while improving environmental quality. Description of research supported by various elements of the materials program is presented below.

THEORETICAL CONDENSED MATTER PHYSICS

The Theoretical Condensed Matter Physics activity provides theoretical support for all parts of the Materials Science and Engineering Division. Research areas include quantum dots, nanotubes and their properties, tribology at the atomic level, superconductivity, magnetism, and optics. A significant effort within the portfolio is the development of advanced computer algorithms and fast codes to treat many-particle systems.

An important facilitating component is the Computational Materials Science Network (CMSN), which enables groups of scientists from DOE laboratories, universities, and (to a lesser extent) industry to address materials problems requiring larger-scale collaboration across disciplinary and organizational boundaries. The FY 2003 funding for this program is $16,993,000 and the DOE contact is Dale D. Koelling, (301) 903-2187.

EXPERIMENTAL CONDENSED MATTER PHYSICS

The portfolio consists of a broad-based experimental program in condensed matter and materials physics research emphasizing electronic structure, surfaces/interfaces, and new materials. It includes the development and exploitation of advanced experimental techniques and methodology. The objective is to provide the understanding of the physical phenomena and processes underlying the properties and behavior of advanced materials. The portfolio includes specific research thrusts in magnetism, semiconductors, superconductivity, materials synthesis and crystal growth, and photoemission spectroscopy. The portfolio addresses well-recognized scientific needs, including understanding magnetism and superconductivity; the control of electrons and photons in solids; understanding materials at reduced dimensionality, including the nanoscale; the physical properties of large, interacting systems; and the properties of materials under extreme conditions. The FY 2003 funding for this program is $37,205,000 and the DOE contact is James Horwitz, (301) 903-4894.

MATERIALS CHEMISTRY AND BIOMOLECULAR MATERIALS

This activity broadly supports basic, exploratory research on the design, synthesis, characterization, and properties of novel materials and structures. The general focus is on the chemical aspects of complex and collective phenomena that give rise to advanced materials. The portfolio emphasizes solid-state chemistry, surface and interfacial chemistry, and materials that underpin many energy-related areas such as batteries and fuel cells, catalysis, friction and lubrication, energy conversion and storage, membranes, electronics and sensors, and materials aspects of environmental chemistry. It includes investigation of novel materials such as low-dimensional solids, self-assembled monolayers, cluster and nanocrystal-based materials, conducting and electroluminescent polymers, organic superconductors and magnets, complex fluids, hybrid materials, biomolecular materials and solid-state neutron detectors. There is an increased emphasis on the synthesis of new materials with nanoscale structural control and taking advantage of unique material properties that originate at the nanoscale. In this regard, addition of a new Program Manager (A. M. K.) for Biomolecular Materials has added a new dimension to the scope of Materials Chemistry research activity. Significant research opportunities exist at the biology/materials science interface since the world of biology offers time-tested strategies and models for the design and synthesis of new materials—composites and molecular assemblies with unique properties and specific functions. A wide variety of experimental techniques are employed to characterize these materials including X-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and X-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as high-resolution magnetic resonance imaging (MRI) without magnets, neutron reflectometry, and surface force apparatus in combination with various spectroscopies. The FY 2003 funding for this program is $40,563,000 and the DOE contacts are Richard Kelley, (301) 903-6051 and Aravinda Kini (301) 903-3565.

MECHANICAL BEHAVIOR AND RADIATION EFFECTS

This activity focuses on understanding the mechanical behavior of materials under static and dynamic stresses and the effects of radiation on materials properties and behavior. The objective is to understand the defectbehavior relationship at an atomic level. In the area of mechanical behavior, the research aims to advance understanding of deformation and fracture and to develop predictive models for design of materials having desired mechanical behavior. In the area of radiation effects, the research aims to advance understanding of mechanisms of amorphization (transition from crystalline to a noncrystalline phase), understand mechanisms of radiation damage, predict and learn how to suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by ion implantation. The FY 2003 funding for this program is $13,323,000 and the DOE contact is Yok Chen, (301) 903-4174.

X-RAY AND NEUTRON SCATTERING

This activity supports basic research in condensed matter and materials physics using neutron and X-ray scattering capabilities primarily at major BES-supported user facilities. Research is aimed at achieving a fundamental understanding of the atomic, electronic, and magnetic properties of materials and their relationship to the physical properties of materials. Both ordered and disordered materials are of interest as are strongly correlated electron systems, surface and interface phenomena, and behavior under environmental variables such as temperature, pressure, and magnetic field. Development of neutron and X-ray instrumentation is a major component of the portfolio. The FY 2003 funding for this program is $37,821,000 and the DOE contact is Helen Kerch, (301) 903-2346.

STRUCTURE AND COMPOSITION OF MATERIALS

Structure and composition of materials includes research on the arrangement and identity of atoms and molecules in materials, specifically the development of quantitative characterization techniques, theories, and models describing how atoms and molecules are arranged and the mechanisms by which the arrangements are created and evolve. Increasingly important are the structure and composition of inhomogeneities including defects and the morphology of interfaces, surfaces, and precipitates. Advancing the state of the art of electron beam microcharacterization methods and instruments is an essential element in this portfolio. Four electron beam user centers are operated at ANL, LBNL, ORNL, and the Frederick Seitz MRL at the University of Illinois. The FY 2003 funding for this program is $28,915,000 and the DOE contact is Altaf Carim, (301) 903-4895.

PHYSICAL BEHAVIOR

Physical behavior refers to the physical response of a material, including the electronic, chemical, magnetic and other properties, to an applied stimulus. The research in this portfolio aims to characterize, understand, predict, and control physical behavior of materials by developing the scientific basis underpin the behavior, and furthermore, establishing rigorous physical models for predicting the response of materials. The form of stimuli ranges from temperature, electrical and magnetic fields, chemical and electrochemical environment, and proximity effects of surfaces or interfaces. Basic research topics supported include characterization of physical properties with an emphasis on the development of new experimental tools and instrumentations, and multi-scale modeling of materials behaviors. Specific areas of research include: electrochemistry and corrosion, high-temperature materials performance, superconductivity, fuel cells, semiconductors/photovoltaics, and more. The FY 2003 funding for this program is $20,262,000 and the DOE contact is Harriet Kung, (301) 903-1330.

SYNTHESIS AND PROCESSING SCIENCES

Synthesis and Processing Science addresses the fundamental understanding necessary to extend from design and synthesis to the preparation of materials with desired structure, properties, or behavior. This includes the assembly of atoms or molecules to form materials, the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and the development of processes to produce materials for specific applications. The goal of basic research in this area ranges from the creation of new materials and the improvement of the properties of known materials, to the understanding of such phenomena as adhesion, diffusion, crystal growth, sintering, and phase transition, and ultimately to the development of novel diagnostic, modeling and processing approaches. This activity also includes development of *in situ* measurement techniques and capabilities to quantitatively determine variations in the energetics and kinetics of growth and formation processes on atomic or nanometer length scales. The FY 2003 funding for this program is $11,839,000 and the DOE contact is Jane Zhu, (301) 903-3811.

ENGINEERING PHYSICS

Engineering Physics advances scientific understanding underlying dynamic interactions of multicomponent systeMs. Areas of emphasis include microscopic and nanoscale science of the interactions of fluid, organic or biological materials with each other and with solid systems and developing the means to advance the characterization of the same. Questions of ongoing interest include, predicting behavior multi-component fluids with and without heat transfer, predicting the behavior of the solid-liquid interface, understanding the interactions of phonons with secondary phases or micro and nanoscale defects in solids, and non-linear behavior of engineering systeMs. The FY 2003 funding for this program is $15,297,000 and the DOE contact is Tim Fitzsimmons, (301) 903-9830.

EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH

Basic research spanning the entire range of programmatic activities supported by the Office of Science in states that have historically received relatively less Federal research funding. The DOE designated EPSCoR states are Alabama, Alaska, Arkansas, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Mexico, North Dakota, Oklahoma, South Carolina, South Dakota, Vermont, West

Virginia, and Wyoming, and the Commonwealth of Puerto Rico. It is anticipated that states of Delaware and Tennessee and US Virgin Islands will become DOE eligible states in FY04. BES manages EPSCoR for the Department. The FY 2003 funding for this program is $11,722,000 and the DOE contact is Matesh Varma, (301) 903-3209.

DIVISION OF SCIENTIFIC USER FACILITIES

X-RAY AND NEUTRON SCATTERING FACILITIES

This activity supports the operation of four synchrotron radiation light sources and three neutron scattering facilities. These are: the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory; the Advanced Photon Source (APS) at Argonne National Laboratory; the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory; the Stanford Synchrotron Radiation Laboratory (SSRL) at Stanford Linear Accelerator Center; the High Intensity Flux Reactor (HFIR) at Oak Ridge National Laboratory; the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory; and the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory. Under construction is the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, which is a nextgeneration short-pulse spallation neutron source that will be significantly more powerful than the best spallation neutron source now in existence—ISIS at the Rutherford Laboratory in England. On the drawing board is the Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center, which is a free-electron laser that will provide laser-like radiation in the X-ray region of the spectrum that is 10 orders of magnitude greater in peak power and peak brightness than any existing coherent Xray light source. The FY 2003 funding for this program is $281,013,000 and the DOE contact is Pedro A. Montano, (301) 903-2347.

NANOSCIENCE CENTERS

This activity supports construction and the subsequent operation of Nanoscale Science Research Centers (NSRCs) at DOE laboratories that already host one or more of the BES major user facilities. Nanotechnology is the creation and use of materials, devices, and systems through the control of matter at the nanometer-length scale, at the level of atoms, molecules, and supramolecular structures. Nanoscience and nanotechnology will fundamentally change the way materials and devices will be produced in the future and subsequently revolutionize the production of virtually every human-made object. Nanoscience will explore and develop the rules and tools needed to fully exploit the benefits of nanotechnology. Each NSRC will combine state-of-the-art equipment for materials nanofabrication with advanced tools for nano characterization. The NSRCs will become a cornerstone of the Nation's nanotechnology revolution, covering the full spectrum of nanomaterials and providing an invaluable resource for universities and industries. The FY 2003 funding for this program is $35,651,000 and the DOE contacts are Kristin A. Bennett, (301) 903-4269 and Altaf Carim, (301) 903-4895.

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

TECHNOLOGY RESEARCH DIVISION

LABORATORY TECHNOLOGY RESEARCH PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING

225. **ADVANCED PROCESSING TECHNIQUES FOR TAILORED NANOSTRUCTURES IN RARE-EARTH PERMANENT MAGNETS (AL 01 02)**
$241,000
DOE Contact: Samuel J. Barish (301) 903-2917
AL Contact: Matthew Kramer (515) 294-0276

High-energy product (BH)max permanent magnets have enabled critical size and weight reduction in direct-current electric motors with an accompanying increase in energy efficiency. Nd-Fe-B based magnets are currently the clear choice for high-value commercial applications. Two classes of magnets are produced from these alloys. While the anisotropic (textured) magnets possess the highest (BH)max, they are limited to critical applications because of their high cost. Bonded magnets made from rapidly solidified alloys have significantly lower (BH)max; but in addition to lower cost of production, they offer the ability to produce net shape magnets and may easily be incorporated in larger motors resulting in considerable energy savings. While considerable progress has been made in controlling the rapid solidification process to reproducibly fabricate high-energy product magnet materials, advances have been largely empirical with limited fundamental understanding. This project supports the DOE mission in advanced synthesis and materials characterization technologies.

Recent developments in high-speed imaging techniques have documented a number of problems regarding the stability of the melt pool during melt spinning, and they provide the tools to address these problems in a systematic manner. A particularly severe problem is the ability of the alloy to wet the quench wheel. When the melt pool fails to wet the quench wheel, the lack of a stable pool will result in lower yield and inhomogeneous solidification of the fraction that contacts the quench wheel. The objective of this project is to determine the factors controlling wettability, including composition, impurities, and heat flow, using imaging techniques. In addition, procedures for processing digital images will be developed so that they may be transferred to the industry partner. The imaging techniques and the resulting enhanced control of processing will also be applied to producing anisotropic rapidly solidified permanent magnet powders. Such powders have the potential to increase the (BH)max of bonded magnets by a factor of four.

Keywords: Permanent Magnets, Anistropic Magnets, Bonded Magnets, (Bh)max, Rapid Solidification Process, High-Speed Imaging Techniques, Quench Wheel, Anisotropic Rapidly Solidified Permanent Magnet Powders

226. **LOW-COST, HIGH-PERFORMANCE YBCO CONDUCTORS (ORNL 01 06)**
$287,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: Parans Paranthaman (
865) 574-5045

The successful demonstration of high-performance YBCO (YBCO) coated conductors by various institutions has generated great interest around the world. This project will support the DOE mission in energy efficiency.

The objective of this project is to develop material science and technology necessary for YBCO coated conductors on biaxially textured, nonmagnetic, high-strength substrates. Fundamental studies of the growth of oxide buffers on these nonmagnetic substrates will be conducted. The research goal is to also develop both vacuum and nonvacuum processes to deposit compatible buffers at high rates. These novel substrates will be the foundation or template upon which the American Superconductor Corporation will apply YBCO using its proprietary trifluoroacetate (TFA) solution process. Applications of these superconducting wires include high-efficiency motors, compact generators, underground transmission lines, oil-free transformers, and superconducting magnetic storage systems for smoothing voltage fluctuations in the power grid. The Rolling Assisted Biaxially Textured Substrates (RABiTS) process developed at ORNL will be utilized. ORNL and ASC have reported a very high J_c of 1.9 MA/cm^2 at 77 K and self-field on YBCO films grown by their TFA solution process on standard RABiTS architecture of CeO_2 (sputtered)/YSZ (sputtered)/Gd_2O_3 (solution)/nickel. However, before scaling up to fabricate long conductors in a reel-to-reel configuration, several fundamental issues will be addressed. Nickel is magnetic, which means significant alternating-current losses, and is also mechanically soft. Hence, the first issue to be addressed is the development of mechanically strong, nonmagnetic, biaxially textured, alloy substrates. The deposition of an epitaxial oxide buffer layer on a nickel-alloy substrate is non-trivial due to the tendency of alloying elements in nickel to form nonepitaxial oxides on the surface of the substrate. The second issue to be addressed is the development of a suitable buffer layer stack for growth of high-J_c YBCO filMs. The high number of buffer layers increases the complexity of fabrication and cost of the conductor. A third objective is to simplify the buffer layer stacks. Because radio frequency magnetron sputtering has limited deposition rates, the fourth issue to be addressed is the investigation of higher rate processes for the fabrication of epitaxial oxide buffer layers on the nonmagnetic substrates. In this project, solutions for critical roadblocks will be addressed to possibly accelerate the development and commercialization of low-cost, YBCO high-temperature superconducting wires.

Keywords: Oxide Buffers, Trifluoroacetate Solution Process, Rabits, Nickel Alloy Substrate, Radio Frequency Magnetron Sputtering

DEVICE OR COMPONENT FABRICATION, BEHAVIOR, OR TESTING

227. **NANOFABRICATION OF ADVANCED DIAMOND TOOLS (LBNL 01 03)**
$221,000
DOE Contact: Samuel J. Barish (301) 903-2917
LBNL Contact: Othon Monteiro (510) 486-6159

This project will investigate and develop fabrication processes for diamond tools and evaluate these tools in actual micromachining operations. The primary use of these tools will be for the repair of masks used in semiconductor processing. No technology is presently available for the repair of defects in masks to be used for the next generations (critical dimension of 0.13 mm and below). Nanomachining can be used for such repairs, and it is regarded as the only technique capable of repairing masks for deep ultraviolet lithography. The diamond tools will be manufactured by plasma-assisted chemical vapor deposition (CVD) of diamond on preformed molds, which are etched off after the deposition is completed. Silicon processing technology will be used to prepare the molds to be filled with diamond. Diamond is the most promising material for such tools because of its superior mechanical properties and wear resistance. This project supports the DOE mission in advanced materials.

The major objective of this project is the development of diamond tools (tips) to be used in micromachining and nanomachining operations using scanning-probe technology. The primary application of these tools will be in the repair of masks for the semiconductor industry. Industry and government groups, such as International Sematech, regard mask repair as absolutely critical to the ability to continue to advance semiconductor performance and device density. LBNL is interested in expanding the applications of CVD diamond to the manufacturing of microsize and nanosize mechanical, electronic, or optical devices. General Nanotechnology is directly interested in bringing the CVD diamond technology to the mask repair tools to be used in the lithography of circuits in the next several generations (critical dimensions below 130 nm). The project team intends to develop a manufacturing process to produce reliable and reproducible diamond tools and fully characterize these tools with regard to their performance in mask repair. The manufacturing process will be based on plasma-assisted CVD on prefabricated molds; for some special applications, final shaping processes will also be developed. The manufacturing process shall be capable of preparing those tool-bits on 4-in. silicon wafers, with diamond deposition rates of 1 to 2 μm/h, which is sufficient to guarantee the economic feasibility of the fabrication technique. In addition, the process shall be able to prepare tools (diamond tips) with different angles of attack and tip radii down to 2 nm. Mechanical toughness and hardness should be optimized, and wear rates of the most common materials used in lithographic masks shall be fully characterized, as well as the wear rate of the tools.

Phase I (Introductory Studies) has been completed. The major parameters affecting nucleation density are the existence of seed layer and the application of bias voltage. A diamond deposition process that makes use of the former has been developed at LBNL and has been used to prepare the initial samples. Implementation of the capability of biasing the substrate is being implemented to the existing diamond deposition chamber: design of the required components (electrodes and vacuum feedthroughs) is under way, and selection and purchase of the power supply are the next steps. The nucleation density achieved with the current process (seed layer) is sufficient to produce continuous (pin-hole free) diamond films with a thickness below 100 nm. Implementation of bias-enhanced nucleation is desired mostly for the capability of producing highly textured diamond filMs. Such films are smoother than conventional polycrystalline filMs. Phases II and III are also progressing at the planned rate. The development of techniques for preparing molds on silicon wafers has been successful. The shift from using conventional silicon to silicon-on-insulator has allowed greater reproducibility in mold and cantilever fabrication. Pyramid molds are currently being fabricated and used to test the diamond deposition process. Concurrently, the scanning-probe instrument that will be used for the evaluation of these nanotools has been installed in LBNL, and final software development is under way to allow the project to begin collecting data on tool performance and wear.

Keywords: Semiconductor Processing, Deep Ultraviolet Lithography, Silicon Processing Technology, Micromachining, Chemical Vapor Deposition, Silicon Wafers, Nucleation Density, Pyramid Molds

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2003 PHASE I

Solid State SPECT Detectors for Molecular Imaging in Small Animals - DOE Contact Peter Kirchner, (301) 903-9106; Photon Imaging, Inc. Contact Dr. Jan S. Iwanczyk, (818) 709-2468

Fast, High Resolution Pet Detector - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

A Remote and Affordable Detection System for Cr(VI) in Groundwater - DOE Contact Michael Kuperberg, (301) 903-3511; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 530-0263

Nanoscale Inorganic Ion-Exchange Films for Enhanced Electrochemical Heavy Metal Detection - DOE Contact Michael Kuperberg, (301) 903-3511; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303)530-0263

SiC/HT-9 MMC Composite Tubes for Fuel Cladding - DOE Contact Madeline Feltus, (301) 903-2308; Accelerator Technology Corporation Contact Dr. Peter McIntyre, (979) 255-5531

Improved Silicon Carbide Materials for Very High-Temperature, Fast-Spectrum Nuclear Energy Systems - DOE Contact Madeline Feltus, (301) 903-2308; Lightweight Solutions, Inc. Contact Dr. T. Dennis Claar, (302) 239-9710

A GEM of a Neutron Detector - DOE Contact Helen Kerch, (301) 903-2346; Instrumentation Associates Contact Dr. R. Berliner, (734) 424-0091

Amorphous, Silicon-Based Neutron Detector - DOE Contact Helen Kerch, (301) 903-2346; Midwest Optoelectronics, LLC Contact Dr. Liwei Xu, (419) 724-0565

Long-Lifetime, Low-Scatter Neutron Polarization Target - DOE Contact Helen Kerch, (301) 903-2346; Science Research Laboratory, Inc. Contact Dr. Jonah Jacob, (617) 547-1122

Polymer White Light Emitting Devices - DOE Contact James Brodrick, (202) 586-1856; Reveo, Inc. Contact Ms. Rayan Faris, (914) 345-9555

Novel Light Extraction Enhancements for OLED Lighting - DOE Contact James Brodrick, (202) 586-1856; Universal Display Corporation Contact Ms. Janice K. Mahon, (609) 671-0980

Molecular-Sieve-Based Nano-Cathode Structures for PEM Fuel Cells - DOE Contact Brian Valentine, (202) 586-1739; Fuelcell Energy, Inc. Contact Mr. Ross M. Levine, (203) 825-6057

Enhanced Optical Efficiency Package Incorporating Nanotechnology Based Downconverter and High Refractive Index Encapsulant for AlInGaN High-Flux White

Led Lamp with High Luminous Efficiency - DOE Contact James Brodrick, (202) 586-1856; Nanocrystals Technology, Ltd. Contact Dr. Rameshwar Bhargava, (914) 923-1142

Efficient Hybrid Phosphors for Blue Solid State Light Emitting Diodes - DOE Contact James Brodrick, (202) 586-1856; Phosphortech Corporation Contact Mr. Christopher J. Summers, (404) 664-5008

Novel, Low - Cost Technology for Solid State Lighting - DOE Contact James Brodrick, (202) 586-1856; Technologies And Devices International, Inc. Contact Dr. V. Dmitriev, (301) 572-7834

Fiber Optic Hydrogen Sensors Based on Nano-sized Metal Alloys - DOE Contact Eric Lightner, (202) 586-8130; Molecular Optoelectronics Corporation Contact Dr. Kevin R. Stewart, (518) 270-8203

Universal Photo-Acoustic Sensor System - DOE Contact Elliott Levine, (6-1476); Physical Optics, Photonic Systems Division Contact Mr. Gordon Drew, (310) 320-3088

Contamination-Resistant Two-Phase Membranes for High-Temperature Hydrogen Separation - DOE Contact Richard J. Dunst, (412) 386-6694; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Real-Time In-Situ Monitoring of Combustion Gas Mixtures by Microporous Solid Array Sensor - DOE Contact Susan Maley, (304) 285-1321; Lynntech, Inc. Contact Dr. G. Duncan Hitchens, (979) 693-0017

Advanced Thermal Spray Fabrication of Solid Oxide Fuel Cells - DOE Contact Shawna Toth, (304) 285-1316; Mesoscribe Technologies, Inc. Contact Mr. Richard Gambino, (631) 444-6455

Low Cost Spray Deposition for SOFC Manufacturing - DOE Contact Shawna Toth, (304) 285-1316; Nextech Materials, Ltd. Contact Mr. William J. Dawson, (614) 842-6066

Low-Cost Rapid Joining for Fabrication/In-Situ Repair of Large SiC Composite Structural Materials for Fusion Reactors and Other Commercial Applications - DOE Contact Gene Nardella, (301) 903-4956; Fm Technologies, Inc. Contact Dr. Frederick Mako, (703) 961-1051

Low-Cost Fabrication of Inertial Fusion Energy Capsule Supports - DOE Contact Gene Nardella, (301) 903-4956; Luxel Corporation Contact Mr. Dan Wittkopp, (360) 378-4137

Microengineered Tungsten Firstwall Structure for Inertial Fusion Energy Reactors - DOE Contact Gene Nardella, (301) 903-4956; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

Design and Testing of a Fast-Release Tilted Target for RIA - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; I. C. Gomes Consulting and Investment, Inc. Contact Dr. Itacil C. Gomes, (630) 640-6189

Microchannel Plate Hard X-Ray Imaging Detector - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Nova Scientific, Inc. Contact Dr. Paul L. White, (508) 347-7679

New N+ Contact for Germanium Strip Detectors - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Ball Grid Array Compatible, Optical Packaging and Assembly Process - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Eltech Precision, Inc. Contact Dr. Matthias Bussmann, (310) 273-4630

Geiger Photodiode Array Readouts for Scintillating Fiber Arrays - DOE Contact Saul Gonzalez, (301) 903-2359; Apeak Contact Dr. Stefan Vasile, (617) 964-1709

Joining of Ceramic Structures for Advanced High Energy Accelerators - DOE Contact Bruce Strauss, (301) 903-3705; Rwbruce Associates, Inc. Contact Dr. Ralph W. Bruce, (410) 757-3333

Extrusion of Tin Hole in Subelements for Internal-Tin Nb_3Sn Superconductor - DOE Contact Bruce Strauss, (301) 903-3705; Accelerator Technology Corporation Contact Dr. Peter McIntyre, (979) 255-5531

A High Current Density, Low Magnetization, Tubular Filamented Nb_3Sn Superconductor - DOE Contact Bruce Strauss, (301) 903-3705; Dsp Alloys Contact Mr. Gordon G. Chase, (858) 274-9228

Development of Internal-Tin Nb/Sn Strand for High Field Accelerator Dipole Applications - DOE Contact Bruce Strauss, (301) 903-3705; Hyper Tech Research, Inc. Contact Mr. Michael Tomsic, (937) 332-0348

Engineered Ceramic Composite Insulators for High Field Magnet Applications - DOE Contact Bruce Strauss, (301) 903-3705; Multiphase Composites Contact Mr. John A. Rice, (303) 684-9242

An Internal Tin Tube Process for High Performance Nb_3Sn Conductors - DOE Contact Bruce Strauss, (301) 903-3705; Supercon, Inc. Contact Mr. Terence Wong, (508) 842-0174

Thermo-Magnetic Continuous Processing of Bi-2212 Cable for HEP - DOE Contact Bruce Strauss, (301) 903-3705; Supercon, Inc. Contact Mr. Terence Wong, (508) 842-0174

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2003 PHASE II (FIRST YEAR)

Perovskite/Oxide Composites as Mixed Protonic/Electronic Conductors for Hydrogen Recovery in IGCC Systems - DOE Contact Arun C. Bose, (412) 386-4467; Ceramatec, Inc. Contact Dr. Michael Keene, (801) 978-2152

Highly Textured Composite Seals for SOFC Applications - DOE Contact Lane Wilson, (304) 285-1336; Nextech Materials, Ltd. Contact Mr. William J. Dawson, (614) 842-6606

Biomimetic Membrane for Carbon Dioxide Capture from Flue Gas - DOE Contact Frank Ferrell, (301) 903-3768; Carbozyme, Inc. Contact Dr. Michael C. Trachtenberg, (609) 499-3600

Low-Cost Nanoporous Sol Gel Separators for Lithium-Based Batteries - DOE Contact Jim Barnes, (202) 586-5657; Optodot Corporation Contact Dr. Steven A. Carlson, (617) 494-9011

New Solid State Lighting Materials - DOE Contact James Brodrick, (202) 586-1856; Maxdem, Inc. Contact Ms. Linda Hope, (909) 394-0644

Transformer Ratio Enhancement Experiment for Next Generation Dielectric Wakefield Accelerators - DOE Contact Bruce Strauss, (301) 903-3705; Euclid Concepts Llc Contact Dr. A.D. Kanereykin, (440) 519-0410

High Current Density (Jc), Low AC Loss, Low Cost Internal-Tin Superconductors - DOE Contact Bruce Strauss, (301) 903-3705; Supergenics Contact Mr. Bruce Zeitlin, (941) 349-0930

Microwave Component Fabrication using the Fast Combustion Driven Compaction Process - DOE Contact Bruce Strauss, (301) 903-3705; Utron, Inc. Contact Dr. F. Douglas Witherspoon, (703) 369-5552

Micro-Photomultiplier Array - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Nanosciences Corporation Contact Dr. Charles Beetz, (203) 267-4440

Electrically Medicated Microetching Manufacturing Process to Replace Emersion and Spray Etching - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Faraday Technology, Inc. Contact Dr. E. Jennings Taylor, (937) 836-7749

Separation and Enrichment of Xenon in Air - DOE Contact Frances Keel , (202) 586-2197; Membrane Technology and Research, Inc. (MTR) Contact Ms. Elizabeth Weiss, (650) 328-2228

High Performance Thermo-Electrically-Cooled LWIR Mercury Cadmium Telluride Detectors - DOE Contact Frances Keel, (202) 586-2197; Fermionics Corporation Contact Dr. C. C. Wang, (805) 582-0155

VEGF-Based Delivery of Boron Therapeutics - DOE Contact Peter Kirchner, (301) 903-9106; Sibtech, Inc. Contact Dr. Joseph M. Backer, (860) 953-1164

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2003 PHASE II (SECOND YEAR)

A High-Power, Ceramic, RF Generator and Extractor - DOE Contact Bruce Strauss, (301) 903-3705; Duly Research, Inc. Contact Dr. David U. L. Yu, (310) 548-7123

KA-Band RF Transmission Line Components for a High-Gradient Linear Accelerator - DOE Contact Bruce Strauss, (301) 903-3705; Omega-p, Inc. Contact Mr. George P. Trahan, (203) 458-1144

A Method to Increase Current Density in a Mono Element Internal Tin Process Superconductor Utilizing ZrO_2 to Refine the Grain Size - DOE Contact Bruce Strauss, (301)903-3705; Supergenics Contact Mr. Bruce Zeitlin, (941) 349-0930

Hermetic Metallization of Aluminum Nitride for Radio Frequency Devices - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Sienna Technologies, Inc. Contact Dr. Canan Savrun, (425) 485-7272

A Liquid-Desiccant Heating/Cooling System Powered by Solar Energy - DOE Contact Lew Pratsch, (202) 586-1512; Ail Research, Inc. Contact Dr. Andrew Lowenstein, (609) 452-2950

Truss-Integrated Thermoformed Ductwork - DOE Contact Esher Kweller, (202) 586-9136; Steven Winter Associates, Inc. Contact Ms. Marie Starnes, (203) 857-0200

Novel Membrane Reactor for the Desulfurization of Transportation Fuels - DOE Contact Charlie Russomanno, (202) 586-7543; Trans Ionics Corporation Contact Sandra C. Schucker, (281) 296-9210

Low Emission Diesel Engines - DOE Contact Charlie Russomanno, (202) 586-7543; Compact Membrane Systems, Inc. Contact Ms. Nadine Cragg--Lester, (302) 999-7996

Low-Cost, Large-Membrane-Area Modules for Gas Separation - DOE Contact Charlie Russomanno, (202) 586-7543; Membrane Technology And Research, Inc. (MTR) Contact Ms. E. G. Weiss, (650) 328-2228

Novel Nano-Structured Catalyst for Steam Gasification of Carbonaceous Feedstocks - DOE Contact Doug Archer, (301) 903-9443; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Amended Silicate Sorbents for Mercury Removal from Flue Gas - DOE Contact Barbara Carney, (304) 285-4671; ADA Technologies, Inc. Contact Mr. Clifton H. Brown, (303) 792-5615

Control of Catalyst Poisons from Coal Gasifiers - DOE Contact Bob Kornosky, (412) 386-4521; TDA Research, Inc. Contact Mr. Michael Karpuk, (303) 940-2301

High-Temperature Highly-Efficient Ceramic Heat Exchanger - DOE Contact Richard J. Dunst, (412) 386-6694; Ceramatec, Inc. Contact Mr. Dale M. Taylor, (801) 978-2132

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2003 PHASE I

A Design of a New Readout Sensor for Spect - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

High Performance Pet Detector - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Enhanced Materials for Reactive Barriers - DOE Contact Justine Alchowiak, (202) 586-4629; Ada Technologies, Inc. Contact Mr. Clifton H. Brown, Jr., (303) 792-5615

Novel Permeable Reactive Barrier Materials for the Mercury Plume - DOE Contact Justine Alchowiak, (202) 586-4629; Lynntech, Inc. Contact Dr. G. Duncan Hitchens, (979) 693-0017

Electrodecontamination for Mitigation of Airborne Contamination - DOE Contact Justine Alchowiak, (202) 586-4629; Ada Technologies, Inc. Contact Mr. Clifton H. Brown, Jr., (303) 792-5615

Improved Method to Convert Coal to Liquid Fuels - DOE Contact Ted Simpson, (301) 903-3913; Hds Consultants, LLC Contact Dr. Harvey D. Schindler, (201) 791-5374

Characterization of Solid Oxide Fuel Cell Components Using Electromagnetic Model-Based Sensors - DOE Contact Lane Wilson, (304) 285-1336; Jentek Sensors, Inc. Contact Dr. Neil J. Goldfine, (781) 642-9666

Harsh-Environment, Fiber-Optic Sensing System for SOFC Applications - DOE Contact Lane Wilson, (304) 285-1336; Luna Innovations, Inc. Contact Ms. Garnett S. Linkous, (540) 953-4274

A Novel Process for the Application and Finishing of Nanocrystalline Superhard Steel onto Internal Combustion Engine Components - DOE Contact Brian Valentine, (202) 586-1739; Faraday Technology, Inc. Contact Dr. E. Jennings Taylor, (937) 836-7749

Evaluation of a Novel Magnetic Activated Carbon Process for Gold Recovery - DOE Contact Michael Canty, (202) 586-8119; Eriez Manufacturing Contact Mr. Chester F. Giermak, (814) 835-6000

Tailorable, Environmental Barrier Coatings for Super- Alloy Turbine Components in Syngas - DOE Contact Udaya Rao, (412) 386-4743; Ceramatec, Inc. Contact Mr. Raymond K. Miller, (801) 978-2114

Hot Section Material Systems Testing and Development for Advanced Power Systems - DOE Contact Udaya Rao, (412) 386-4743; Florida Turbine Technologies, Inc. Contact Mrs. Shirley Coates Brostmeyer, (561) 746-3317

Advanced Thermal Barrier Coatings for Turbine Components - DOE Contact Udaya Rao, (412) 386-4743; Mer Corporation (Materials And Electrochemical Res) Contact Dr. James C. Withers, (520) 574-1980

SiCN High Temperature Microelectromechanical Systems (MEMS) Sensor Suite - DOE Contact Susan Maley, (304) 285-1321; Sporian Microsystems, Inc. Contact Mr. Wenge Zhang, (303) 516-9075

Enhanced Performance Carbon Foam Heat Exchanger for Power Plant Cooling - DOE Contact Barbara Carney, (304) 285-4671; Ceramic Composites, Inc. Contact Mrs. Sharon Fehrenbacher, (410) 224-3710

Selective Adsorption Membranes for Natural Gas Upgrading - DOE Contact Tony Zammerilli, (304) 285-4641; ITN Energy Systems, Inc. Contact Ms. Janet Casteel, (303) 285-5111

Dehydration of Natural Gas - DOE Contact Tony Zammerilli, (304) 285-4641; Membrane Technology and Research, Inc. Contact Ms. Elizabeth Weiss, (650) 328-2228

Membranes for Methane/Nitrogen Seperation - DOE Contact Tony Zammerilli, (304) 285-4641; Membrane Technology and Research, Inc. Contact Ms. Elizabeth Weiss, (650) 328-2228

High Pressure Economical Process for Treating Natural Gas - DOE Contact Tony Zammerilli, (304) 285-4641; TDA Research, Inc. Contact Mr. John D. Wright, (303) 940-2300

A Novel Oxidation Process for the Conversion of Coal to Diesel Fuel-Grade Chemicals - DOE Contact Ted Simpson, (301) 903-3913; Ceramem Corporation Contact Dr. Richard J. Higgins, (781) 899-4495

Novel Fischer-Tropsch Reactor - DOE Contact Kathy Stirling, (918) 699-2008; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Innovative Inorganic Fusion Magnet Insulation Systems - DOE Contact Warren Marton, (301) 903-4956; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Vacuum Pressure Impregnation Insulation Systems for High Temperature Fusion Applications - DOE Contact Warren Marton, (301) 903-4956; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Thermomechanical Processing of Nb for Improved Superconductor Applications - DOE Contact Warren Marton, (301) 903-4956; Shear Form Contact Dr. K.T. Harwig, (979) 693-4102

Preceramic Precursor Routes to Tailorable, Low-Activation, Silicon-Carbide-Based Joints - DOE Contact Sam E. Berk, (301) 903-4171; Ceramatec, Inc. Contact Dr. Balky Nair, (801) 956-1000

An Advanced Monolithic NbTi Conductor with 5 Tesla Jc of 5000 A/mm^2 and Beyond for Use in Superconducting Quadrupole Magnets - DOE Contact Francis Thio, (301) 903-4678; Supercon, Inc. Contact Mr. Terence Wong, (508) 842-0174

Aluminum Nitride Radio Frequency Windows - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Sienna Technologies, Inc. Contact Dr. Ender Savrun, (425) 485-7272

A New SRF Cavity Processing Technique for the Elimination of Field Emission and Surface Preparation in Fully Assembled Cavities - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Avar, Inc. Contact Ms. Roisin Preble, (757) 595-4643

A Novel Design for CZT Gamma Ray Spectrometers - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Compact Surface Mount Miniature Photomultipliers - DOE Contact Michael P. Procario, (301) 903-2890; Nanosciences Corporation Contact Mr. William H. Overholt, (203) 267-4440

Some Improved Methods of Introducing Additional Elements into Internal-tin Nb_3Sn - DOE Contact Bruce Strauss, (301) 903-3705; Supergenics, Llc Contact Mr. Bruce Zeitlin, (941) 349-0930

Fast X-Band Phase Shifter - DOE Contact Bruce Strauss, (301) 903-3705; Omega-p, Inc. Contact Dr. George P. Trahan, (203) 789-1164

Near Net Shape Manufacturing Using Combustion Driven Compaction - DOE Contact Bruce Strauss, (301) 903-3705; Utron, Inc. Contact Dr. F. Douglas Witherspoon, (703) 369-5552

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2003 PHASE II (FIRST YEAR)

Multilayer Composite Membranes for Upgrading Acid-Rich Natural Gas - DOE Contact Tony Zammerilli, (304) 285-4641; Membrane Technology and Research, Inc. (MTR) Contact Ms. Elizabeth Weiss, (650) 328-2228

Stabilized Lithium Manganese Oxide Spinel Cathode for High Power Li-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Farasis Energy, Inc. Contact Dr. Keith D. Kepler, (650) 594-4380

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2003 PHASE II (SECOND YEAR)

Doppler Laser Radar for Non-Intrusive Liquid Metal Flow Characterization - DOE Contact Gene Nardella, (301) 903-4956; Think Tank, Inc. Contact Dr. Madhavan M. Menon, (865) 966-6200

Multi-Megawatt Circulator for TE01 Waveguide - DOE Contact Bruce Strauss, (301) 903-3705; Calabazas Creek Research Contact Dr. Lawrence Ives, (408) 741-8680

Active Vibration Control of NLC Magnets - DOE Contact Bruce Strauss, (301) 903-3705; Energen, Inc. Contact Dr. Chad H. Joshi, (978) 671-5400

An Electrical Condition Monitoring Approach for Wire and Cable - DOE Contact Frank Ross, (301) 903-4416; BPW Incorporated Contact Mr. Shelby J. Morris Jr., (757) 850-8679

X-Ray Diagnostics for High-Temperature Superconductor Processing - DOE Contact David Welch, (631) 344-3517; Aracor Contact Mr. Ed LeBaker, (408) 733-7780

Non-Invasive Techniques to Study Local Passivity Breakdown of Metal Alloys in Aqueous Media - DOE Contact Kevin Zavadil, (505) 845-8442; Applicable Electronics, Inc. Contact Mr. Alan M. Shipley, (508) 833-5042

Microelectrode Array for Electrochemical Sensing of Localized Corrosion - DOE Contact Kevin Zavadil, (505) 845-8442; Faraday Technology, Inc. Contact Dr. E. Jennings Taylor, (937) 836-7749

Intelligent Probes for Enhanced Non-Destructive Determination of Degradation in Hot-Gas-Path Components - DOE Contact Lane Wilson, (304) 285-1336; Jentek Sensors, Inc. Contact Dr. Neil J. Goldfine, (781) 642-9666

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2003 PHASE I

Al(In)GaN-Based, High-Electron Mobility Transistors (HEMTs) on SiC for High-Power Radar Applications - DOE Contact Vaughn Standley, (202) 586-1874; SVT Associates Contact Ms. Janes Marks, (952) 934-2100

Cell-Free Protein Synthesis for High-Through-Put Proteomics - DOE Contact Marvin Stodolsky, (301) 903-4475; Macconnell Research Corporation Contact Dr. William P. MacConnell, (858) 452-2603

A New Class of Trimetasphere Based Radiopharmaceuticals - DOE Contact Prem Srivastava, (301) 903-4071; Luna Innovations, Inc. Contact Ms. Garnett S. Linkous, (540) 953-4274

Low-Cost Automatic Tool Fixturing Based on Dexterous Robotic Hand - DOE Contact Justine Alchowiak, (202) 586-4629; Barrett Technology, Inc. Contact Mr. Burt Doo, (617) 252-9000

Nanoengineered ODS Feritic/Martensitic Steel for Fusion Application - DOE Contact Madeline Feltus, (301) 903-2308; Powdermet, Inc. Contact Mr. Andrew J. Sherman, (216) 404-0053

Low-Porosity SiC/SiC Composite Materials for Nuclear Energy System Components - DOE Contact Madeline Feltus, (301) 903-2308; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

Solid-State Thermal-Neutron Detector Based on Boron-Doped a-Se Stabilized Alloy Films - DOE Contact Helen Kerch, (301) 903-2346; Eic Laboratories, Inc. Contact Dr. R. David Rauh, (781) 769-9450

New, Stable Cathode Materials for OLEDs - DOE Contact James Brodrick, (202) 586-1856; International Technology Exchange, Inc. Contact Dr. Terje Skotheim, (520) 299-9533

Novel Lower-Voltage OLEDs for Higher-Efficiency Lighting - DOE Contact James Brodrick, (202) 586-1856; Universal Display Corporation Contact Ms. Janice K. Mahon, (609) 671-0980

Nanowire Cathode Material for Lithium-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Boundless Corporation Contact Dr. Timothy L. Feaver, (303) 664-9962

High Performance Solid Polymer Electrolyte for Lithium Batteries - DOE Contact Jim Barnes, (202) 586-5657; Mer Corporation (materials And Electrochemical Res Contact Dr. Raouf O. Loutfy, (520) 574-1980

Multi-Layer Anode Stabilization Layer For Preventing Dendrites and Li Corrosion In Lithium-Sulfur Batteries - DOE Contact Jim Barnes, (202) 586-5657; Sion Power Corporation Contact Dr. James R. Akridge, (520) 799-7516

Highly Conductive Solvent-Free Polymer Electrolytes for Lithium Rechargeable Batteries - DOE Contact Jim Barnes, (202) 586-5657; Techdrive, Inc. Contact Dr. Robert Filler, (312) 567-3910

$LiFePO_4$ Cathode Material Designed for Use in Lithium-Ion Batteries with Application to Electric and Hybrid-Electric Vehicles - DOE Contact Jim Barnes, (202) 586-5657; Tiax, LLC Contact Ms. Renee Wong, (617) 498-5655

Preparation of High Performance Nanocomposite Cathode Materials - DOE Contact Jim Barnes, (202) 586-5657; TPL, Inc. Contact Mr. Harold M. Stoller, (505) 342-4412

High Energy Density Rechargeable Lithium Sulfur Battery with Novel Solid Electrolyte - DOE Contact Jim Barnes, (202) 586-5657; U. S. Nanocorp, Inc. Contact Dr. David E. Reisner, (860) 678-7561

Polysiloxane-Transition Metal Complex Copolymer Catalysts for Asymmetric Transformations - DOE Contact Charlie Russomanno, (202) 586-7543; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 530-0263

Metal Oxide Catalyst for Methyl Ethyl Ketone Production via One-Step Oxidation of n-Butane - DOE Contact Charlie Russomanno, (202) 586-7543; Evernu Technology, LLC Contact Dr. Manhua Mandy Lin, (215) 659-8574

Discovery and Optimization of New Heterogeneous Catalysts for the Direct Production of Propylene Oxide (PO) from Propylene and Oxygen Using Combinatorial Methods - DOE Contact Charlie Russomanno, (202) 586-7543; Laboratory Catalysts Systems, Llc Contact Mr. Craig Leidholm, (310) 216-7079

Nano-Zeolite Coatings on Microlith Substrates for High Selectivity Chemical Reactions - DOE Contact Charlie Russomanno, (202) 586-7543; Precision Combustion, Inc. Contact Mr. Paul Donahe, (203) 287-3700

Novel Catalytic Technology for Propylene Epoxidation - DOE Contact Charlie Russomanno, (202) 586-7543; Ceramem Corporation Contact Dr. Richard J. Higgins, (781) 899-4495

New Nanostructured Polymeric Membrane for Direct Methanol Fuel Cells - DOE Contact Charlie Russomanno, (202) 586-7543; Icet, Inc. Contact Dr. Srinivasan Sarangapani, (781) 769-6064

Low Cost and High Performance, Polymer Nanocomposite, Specialty Industrial Coatings - DOE Contact Charlie Russomanno, (202) 586-7543; Nei Corporation Contact Dr. Gary Tompa, (732) 885-1088

PET Nanocomposites for Beverage Container Applications - DOE Contact Charlie Russomanno, (202) 586-7543; TDA Research, Inc. Contact Mr. John D. Wright, (303) 940-2302

Ultra-Hard Nanostructured Silicon Carbide for Deep-Hole Drilling - DOE Contact Brian Valentine, (202) 586-1739; Hyper-therm High-temperature Composites, Inc. Contact Mr. Wayne S. Steffier, (714) 375-4085

Industrial Nano Material Components with High Temperature Corrosion and Wear Resistance Performance for Energy Savings - DOE Contact Brian Valentine, (202) 586-1739; Iap Research, Inc. Contact Dr. John P. Barber, (937) 296-1806

A New Composite Proton Exchange Membrane - DOE Contact Brian Valentine, (202) 586-1739; Lynntech, Inc. Contact Dr. G. Duncan Hitchens, (979) 693-0017

CCVD-Produced, Oxygen-Deficient, Nanocrystalline Perovskite for Low-Temperature Proton Exchange Membranes - DOE Contact Brian Valentine, (202) 586-1739; nGimat Company Contact Mr. John G. Edwards, (678) 287-2445

High Temperature-Stable Membrane Electrode Assemblies for Fuel Cells Fabricated via Ink Jet Deposition - DOE Contact Brian Valentine, (202) 586-1739; Nanosonic, Inc. Contact Dr. Richard O. Claus, (540) 953-1785

Membrane Separation Combined with Catalytic Biomass Gasification to Produce Hydrogen-Rich Gas - DOE Contact Mark Decot, (202) 586-6501; Metcon Industries Contact Mr. Bob Metgud, (856) 722-5600

UV LEDs for Solid State Lighting - DOE Contact James Brodrick, (202) 586-1856; Cermet, Inc. Contact Mr. Jeff E. Nause, (404) 351-0005

Efficient Incandescent Visible Light Produced by Improved Boride and Nitride Filament Radiation - DOE Contact James Brodrick, (202) 586-1856; Foster-Miller, Inc. Contact Mr. Ross R. Olander, (781) 684-4183

Gallium-Nitride Substrates for Improved, Solid-State Lighting - DOE Contact James Brodrick, (202) 586-1856; Kyma Technologies, Inc. Contact Mr. Edward Pupa, (919) 789-8880

An Optical Fiber Probe for the Measurement of High Temperatures - DOE Contact Elliott Levine, (6-1476); Hope Technologies, Inc. Contact Dr. Edelgard Morse, (617) 358-1035

Cost Effective Improved Refractory Materials for Gasification Systems - DOE Contact Jenny Tennant, (304) 285-4830; Blasch Precision Ceramics, Inc. Contact Mr. John R. Parrish, (518) 436-1263

Dense Membrane for Hydrogen Separation Based on High Proton Conductivity and Chemical Stability - DOE Contact Richard J. Dunst, (412) 386-6694; U. S. Nanocorp, Inc. Contact Dr. David E. Reisner, (860) 678-7561

Development of Protective Coatings for Single-Crystal Turbine Blades - DOE Contact Udaya Rao, (412) 386-4743; Ues, Inc. Contact Mr. Francis F. Williams, Jr., (937) 426-6900

Advanced Net-Shape Insulation for Solid Oxide Fuel Cells - DOE Contact Travis Shultz, (304) 285-1370; Ceramatec, Inc. Contact Mr. Raymond K. Miller, (801) 978-2144

High-Performance, Plasticization-Resistant Membranes for Natural Gas Separations - DOE Contact Tony Zammerilli, (304) 285-4641; Membrane Technology and Research, Inc. Contact Ms. Elizabeth Weiss, (650) 328-2228

Cost Effective Fischer-Tropsch Technology - DOE Contact Kathy Stirling, (918) 699-2008; Exelus, Inc. Contact Mr. Mitrajit Mukherjee, (973) 740-2350

Nanocomposite Dielectric Materials for High Frequency Applications - DOE Contact T. V. George, (301) 903-4957; Tpl, Inc. Contact Mr. Harold M. Stoller, (505) 342-4412

Combinatorial Strategy Toward Fast and Efficient Scintillators - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Lutronics, Inc. Contact Mrs. Ling Li, (978) 244-0881

Very Large, High Gain APDs for Particle Physics - DOE Contact Saul Gonzalez, (301) 903-2359; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2003 PHASE II (FIRST YEAR)

Embedded Sensors in Turbine Systems by Direct Write Thermal Spray Technology - DOE Contact Charles T. Alsup, (304) 284-5432; Mesoscribe Technologies, Inc. Contact Mr. Richard Gambino, (631) 632-9513

Catalyst to Improve Small-Scale Claus Plants - DOE Contact Tony Zammerilli, (304) 285-4641; Tda Research, Inc. Contact Mr. John D. Wright, (303) 940-2300

LSGM Based Composite Cathodes for Anode Supported, Intermediate Temperature (600-800 degrees C) Solid Oxide Fuel Cells (SOFC) - DOE Contact Lane Wilson, (304) 285-1336; Materials and Systems Research, Inc. Contact Dr. Dinesh K. Shetty, (801) 530-4987

Metal Oxide Catalyst for Methacrylic Acid Preparation via One-Step Oxidation of Isobutane - DOE Contact Charlie Russomanno, (202) 586-7543; Evernu Technology, LLC Contact Dr. Manhua Mandy Lin Ph.D, (215) 649-8574

P-Type ZnO Films - DOE Contact Satyen Deb, (303) 384-6405; Structured Materials Industries, Inc. Contact Dr. Gary S. Tompa, (732) 885-5909

An Advanced Cathode Material for Li-Ion Battteries - DOE Contact Jim Barnes, (202) 586-5657; A123 Systems Contact Mr.Ric Fulop, (617) 250-0565

Three-Dimension Woven Carbon-Glass Hybrid Wind Turbine Blades - DOE Contact John Cadogan, (202) 586-1991; 3tex, Inc. Contact Mr. R. Bradley Lienhart, (919) 481-2500

Feasibility of Cost Effective, Long Length, BSCCO 2212 Round Wires, for Very High Field Magnets, Beyond 12 Tesla at 4.2 Kelvin - DOE Contact Bruce Strauss, (301) 903-3705; Superconductive Components, Inc. Contact Mr. J.R. Gaines, Jr., (614) 486-0261

Growth of a New, Fast Scintillator Crystal for Nuclear Experiments - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Ceramare Corporation Contact Dr. Larry E. McCandlish, (732) 937-8260

A New Scintillator for Gamma Ray Spectroscopy - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Diamond Windows for High Power Microwave Transmission - DOE Contact T. V. George, (301) 903-4957; Coating Technology Solutions, Inc. Contact Dr. Roy Gat, (617) 625-2725

Radiation Resistant Insulation with Improved Shear Strength for Fusion Magnets - DOE Contact Warren Marton, (301) 903-4958; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Nanostructured Tungsten for Improved Plasma Facing Component Performance - DOE Contact Gene Nardella, (301) 903-4956; Plasma Processes, Inc. Contact Mr. Timothy McKechnie, (256) 851-7653

Low Cost Materials for Neutron Absorption in Generation IV Nuclear Power Systems - DOE Contact Madeline Feltus, (301) 903-2308; Powdermet, Inc. Contact Mr. Andrew Sherman, (818) 768-6420

High Resolution Gamma Ray Spectrometer for Nuclear Non-Proliferation - DOE Contact Frances Keel, (202) 586-2197; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Growth of a New Mid-IR Laser Crystal - DOE Contact Frances Keel, (202) 586-2197; Ceramare Corporation Contact Dr. Larry E. McCandlish, (732) 937-8260

Induim Arsenide Antimonide Very Long Wavelength Photodiodes for Near Room Temperature Operation - DOE Contact Frances Keel, (202) 586-2197; SVT Associates Contact Ms. Jane Marks, (952) 934-2100

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2003 PHASE II (SECOND YEAR)

Innovative Organic and Inorganic High-Pressure Laminate Insulation for Fusion and Superconducting Magnets - DOE Contact Warren Marton, (301) 903-4958; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Inorganic-Organic Hybrid Materials: Diacetylene-Siloxanes as Radiation Resistant Electrical Insulator for Plasma Fusion Confinement Systems - DOE Contact Warren Marton, (301) 903-4958; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 530-0263

Ultra-Thin Optical Diagnostic Filters for Plasma Wakefield Accelerators - DOE Contact Bruce Strauss, (301) 903-3705; Luxel Corporation Contact Mr. Dan Wittkopp, (360) 378-4137

Enhanced Efficiency Nanowire Photocathode for Large PMTs - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Nanosciences Corporation Contact Dr. John Steinbeck, (203) 267-4440

Superinsulation for Ductwork - DOE Contact Esher Kweller, (202) 586-9136; Aspen Aerogels, Inc. Contact Dr. Kang P. Lee, (508) 481-5058

Recycling of Coated Plastics Used in Automotive, IT and Commercial Applications - DOE Contact Charlie Russomanno, (202) 586-7543; Metss Corporation Contact Dr. Kenneth J. Heater, (614) 842-6600

Two-Step Methane Conversion to Alkynes and Dienes - DOE Contact Charlie Russomanno, (202) 586-7543; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Improved Buffered Substrates for YBCO Coated Conductors - DOE Contact David Welch, (631) 344-3517; American Superconductor Corporation Contact Mr. Thomas M. Rosa, (508) 621-4265

Low Cost MesoCarbon Micro Bead Anodes for Lithium-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Mer Corp (materials And Electrochemical Research) Contact Dr. J.C. Withers, (520) 574-1980

A Novel Cathode Material for High Power Lithium Rechargeable Batteries - DOE Contact Jim Barnes, (202) 586-5657; T/j Technologies, Inc. Contact Mr. Leslie Alexander, (734) 213-1637

Development of Low-Cost Salts for Lithium-Ion, Rechargeable Batteries - DOE Contact Jim Barnes, (202) 586-5657; Yardney Technical Products, Inc. Contact Mr. Vince Yevoli, (860) 599-1100

High-Performance Carbon Materials for Ultracapacitors - DOE Contact Ben Hsieh, (304) 285-4254; Advanced Fuel Research, Inc. Contact Dr. Michael A. Serio, (860) 528-9806

Synthesis of Bulk Amounts of Double-Walled Carbon Nanotubes - DOE Contact Ben Hsieh, (304) 285-4254; Mer Corp (materials And Electrochemical Research) Contact Dr. J. C. Withers, (520) 574-1980

Intermediate Temperature Solid Oxide Fuel Cell Development - DOE Contact Lane Wilson, (304) 285-1336; Ceramatec, Inc. Contact Dr. Michael Keene, (801) 978-2152

Novel Ceria-Based Materials for Low-Temperature Solid Oxide Fuel Cells - DOE Contact Lane Wilson, (304) 285-1336; Nextech Materials, Ltd. Contact Dr. Scott L. Swartz, (614) 842-6606

INSTRUMENTATION AND FACILITIES

FY 2003 PHASE I

Situational Awareness Monitor for Nuclear Events - DOE Contact Frances Keel, (202) 586-2187; ADA Technologies, Inc. Contact Mr. Clifford H. Brown, Jr., (303) 792-5615

Low-Noise Borehole Triaxial Seismometer - DOE Contact Frances Keel, (202) 586-2197; Geotech Instruments, LLC Contact Dr. Lani Oncescu, (214) 221-0000

Compact, Short-Pulse Laser Source for Active Imaging Systems - DOE Contact Frances Keel, (202) 586-2197; Aculight Corporation Contact Dr. Dennis Lowenthal, (425) 482-1100

Advanced, Aerosol Mass Spectrometer for Aircraft Measurement of Organic Particulate Matter - DOE Contact Michael Huesemann, (360) 681-3618; Aerodyne Research, Inc. Contact Dr. Charles E. Kolb, (978) 663-9500

Cavity Attenuation Phase Shift Spectroscopic Detection of Nitrogen Dioxide - DOE Contact Michael Huesemann, (360) 681-3618; Aerodyne Research, Inc. Contact Dr. Charles E. Kolb, (978) 663-9500

Novel Ultrasensitive Instrumentation for Trace Gas Measurements in the Field - DOE Contact Michael Huesemann, (360) 681-3618; Los Gatos Research Contact Ms. Noel Wong O'Keefe, (650) 965-7780

NO_2- Sensor for Urban and Regional Air Quality Monitoring - DOE Contact Michael Huesemann, (360) 681-3618; Novawave Technologies Contact Dr. James J. Scherer, (650) 341-3948

Fiber-Laser-Based Water Vapor Differential Absorption Lidar System - DOE Contact Michael Huesemann, (360) 681-3618; Sigma Space Corporation Contact Dr. J. Marcos Sirota, (301) 552-6300

Innovative Carbon Dioxide Sensor Based on Cavity Ringdown - DOE Contact Roger Dahlman, (301) 903-4951; Picarro, Inc. Contact Mr. Tom Oswold, (408) 470-6099

High Precision CO_2 Sensor for Balloon Sonde Atmospheric Measurements - DOE Contact Roger Dahlman, (301) 903-4951; Southwest Sciences, Inc. Contact Dr. Alan C. Stanton, (505) 984-1322

Innovative Instrumentation and Intelligent Diagnostic System for Reactor Safety - DOE Contact Madeline Feltus, (301) 903-2308; En'urga, Inc. Contact Mrs. Deepa Divakaran, (765) 497-3269

Real-Time Monitoring of Catalytic Surfaces for Petrochemical Synthesis Using a Mass/Heat Flow Sensor - DOE Contact Charlie Russomanno, (202) 586-7543; Masscal Corporation Contact Dr. Allan L. Smith, (508) 241-8628

A Down-Hole Probe for Real-Time Ore Grade Assessment in "Look Ahead" Mining - DOE Contact Michael Canty, (202) 586-8119; Resonon, Inc. Contact Dr. Michael R. Kehoe, (406) 586-3356

Development of HSTAT for HVAC Health Status and Control - DOE Contact Terrence Logee, (202) 586-1689; Steven Winter Associates, Inc. Contact Mr. Steven Winter, (203) 857-0200

First-Ever Mobile System for In Situ Acquisition of Isotope Data on Natural Gas - DOE Contact Jim Ammer, (304) 285-4383; In Situ Isotope Services, Inc. Contact Mr. Richard A. Socki, (716) 818-7544

Low-Cost Distributed Sensing for Gas Pipelines - DOE Contact Richard Baker, (304) 285-4714; Ipitek Contact Mr. Robert Downey, (760) 438-1010

A Reliable Optical System for Natural Gas Pipeline Leak Detection - DOE Contact Daniel Driscoll, (304) 285-4717; Southwest Sciences, Inc. Contact Dr. Alan C. Stanton, (505) 984-1322

Downhole Spectrometric Device for the Real-Time Analysis of Fluid Composition - DOE Contact Daniel Ferguson, (918) 699-2047; Hanby Environmental Laboratory Procedures, Inc. Contact Mr. John D. Hanby, (281) 391-4257

An Extremely High Power, Field-Coupled, Low-Loss RF Transmission Line for SRF Cavities - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Avar, Inc. Contact Ms. Roisin Preble, (757) 595-4643

Magnetized Electron Transport in the Proposed Electron Cooling Section of the Relativistic Heavy Ion Collider - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Tech-x Corporation Contact Dr. John R. Cary, (303) 448-0727

Ultra High Speed Analog to Digital Converter with Ternary Digital Output - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Advanced Science And Novel Technology Company Contact Dr. Vladimir Katzman, (310) 377-6029

Pulse-Synchronized Serializer/De-Serializer-Based Interconnect - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Eltech Precision, Inc. Contact Dr. Matthias Bussmann, (310) 273-4630

New Hybrid Pulse-Processor for X- and Gamma-Ray Spectroscopy - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Photon Imaging, Inc. Contact Dr. Bradley E. Patt, (818) 709-2468

Digital Signal Processing Electronics for Nuclear Physics Applications - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Skutek Instrumentation Contact Ms. Joanna Klima, (585) 256-0842

High-Speed Centralized Intrusion Detection Device - DOE Contact Thomas Ndousse-Fetter, (301) 903-9960; Eltech Precision, Inc. Contact Dr. Mattias Bussmann, (310) 273-4630

High Speed Optical Source for High Energy Physics Data Acquisition - DOE Contact Saul Gonzalez, (301) 903-2359; Photodigm, Inc. Contact Mr. Jack Mattis, (972) 235-7584

High Precision, Integrated Beam Position and Emittance Monitor - DOE Contact Bruce Strauss, (301) 903-3705; Far-tech, Inc. Contact Mr. Jin-Soo Kim, (858) 455-6655

Six-Dimensional Beam Cooling in a Gas Absorber - DOE Contact Bruce Strauss, (301) 903-3705; Muons, Inc. Contact Ms. Linda L. Even, (757) 930-1463

Electron Bunch Length Diagnostic Device - DOE Contact Bruce Strauss, (301) 903-3705; Omega-p, Inc. Contact Dr. George P. Trahan, (203) 789-1164

High-Power Radio Frequency Window - DOE Contact Bruce Strauss, (301) 903-3705; Asgard Microwave Contact Mr. David B. Aster, (509) 534-5011

Sheet Beam Klystron for Accelerators - DOE Contact Bruce Strauss, (301) 903-3705; Calabazas Creek Research Contact Dr. Purobi Phillips, (650) 400-5698

Hybrid Modulator Upgrade - DOE Contact Bruce Strauss, (301) 903-3705; Diversified Technologies, Inc. Contact Mr. Michael A. Kempkes, (781) 275-9444

NLC Marx Bank Modulator - DOE Contact Bruce Strauss, (301) 903-3705; Diversified Technologies, Inc. Contact Mr. Michael A. Kempkes, (781) 275-9444

Quasi-Optical 34-GHz Radio Frequency (RF) Pulse Compressor - DOE Contact Bruce Strauss, (301) 903-3705; Omega-p, Inc. Contact Dr. George P. Trahan, (203) 789-1164

KA-Band Resonant Ring for High-Power Testing of Accelerator Components - DOE Contact Bruce Strauss, (301) 903-3705; Omega-p, Inc. Contact Dr. George P. Trahan, (203) 789-1164

A Hydrostatic Processing Facility for Superconducting Wire - DOE Contact Bruce Strauss, (301) 903-3705; Alabama Cryogenic Engineering, Inc. Contact Ms. Mary T. Hendricks, (256) 536-8629

Novel Magnetometer for Quadrupole and Dipole Magnetic Measurements - DOE Contact Bruce Strauss, (301) 903-3705; Tai-Yang Research Corporation Contact Dr. Christopher M. Rey, (302) 494-4048

Development of Sub-Picosecond Phase Stability Signal Multipliers - DOE Contact Bruce Strauss, (301) 903-3705; Wenzel Associates, Inc. Contact Ms. Liz Ronchetti, (512) 450-1400

INSTRUMENTATION AND FACILITIES

FY 2003 PHASE II (FIRST YEAR)

An Inexpensive, Efficient Neutron Monochromator - DOE Contact Helen Kerch, (301) 903-2346; Adelphi Technology, Inc. Contact Dr. Charles K. Gary, (650) 328-7337

High Gain, Fast Scan, Broad Spectrum, Parallel Beam Wavelength Dispersive X-Ray Spectrometer for SEM - DOE Contact Dean Miller, (630) 252-4108; Parallax Research, Inc. Contact Mr. David Ohara, (850) 580-5481

Advanced X-Ray Detectors for Transmission Electron Microscopy - DOE Contact Dean Miller, (630) 252-4108; Photon Imaging, Inc. Contact Dr. Bradley E. Patt, (818) 709-2468

Using Convergent Beams for Small-Sample, Time-of-Flight Neutron Diffraction - DOE Contact Helen Kerch, (301) 903-2346; X-ray Optical Systems, Inc. Contact Mr. David Usher, (518) 464-3334

INSTRUMENTATION AND FACILITIES

FY 2003 PHASE II (SECOND YEAR)

Sol-Gel Derived Neutron Detector Using a Lithiated Glass - DOE Contact Helen Kerch, (301) 903-2346; Neutron Sciences, Inc. Contact Mr. Andrew Stephan, (865) 523-0775

Development of an Ultra-Bright Electron Source for Scanning Transmission Electron Microscopy - DOE Contact Dean- miller@anl.com Mill, (630) 252-4108; Nion Co. Contact Mr. G. J. Corbin, (425) 576-9060

Pixel-Cell Neutron Detector and Read-Out System Meeting Requirements of Present and Future Neutron Scattering Facilities - DOE Contact Helen Kerch, (301) 903-2346; Ordela, Inc. Contact Mr. Daniel M. Kopp, (865) 483-8675

Novel Neutron Detector for High Rate Imaging Applications - DOE Contact Helen Kerch, (301) 903-2346; Proportional Technologies, Inc. Contact Dr. Jeffrey L. Lacy, (713) 747-7324

MATERIALS STRUCTURE AND COMPOSITION

FY 2003 PHASE II (FIRST YEAR)

Development of a New, Low Frequency, Rf-Focused Linac Structure - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Linac Systems Contact Mrs. Barbara C. Swenson, (505) 798-1904

SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2003 PHASE I

Engineered Tungsten Surfaces for IFE Dry Chamber Walls - DOE Contact Gene Nardella, (301) 903-4956; Plasma Processes, Inc. Contact Mr. Timothy McKechnie, (856) 851-7653

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2003 PHASE II (FIRST YEAR)

Carbon Fiber Composite Aeroelastically Tailored Rotor Blades for Utility-Scale Wind Turbines - DOE Contact John Cadogan, (202) 586-1991; K. Wetzel & Company Contact Dr. Kyle K. Wetzel, (785) 766-2450

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2003 PHASE II (SECOND YEAR)

Advanced Membrane Technology for Biosolvents - DOE Contact Charlie Russomanno, (202) 586-7543; Vertec Biosolvents, Inc. Contact Mr. James E. Opre, (847) 803-0575

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2003 PHASE I

Improved Electron Yield and Spin-Polarization from III-V Photocathodes via Bias Enhanced Carrier Drift - DOE Contact Jerry Peters, (301) 903-3233; Nanohmics, Inc. Contact Dr. Keith D. Jamison, (512) 349-0835

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2003 PHASE II (FIRST YEAR)

Hydroforming of Light Weight Components from Aluminum and Magnesium Sheet and Tube - DOE Contact Mike Kassner, (541) 737-7023; Applied Engineering Solutions, LLC Contact Mr. David Guza, (614) 789-9890

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2003 PHASE II (SECOND YEAR)

Neutron Scattering Instrumentation for Measurement of Melt Structure - DOE Contact Helen Kerch, (301) 903-2346; Containerless Research, Inc. Contact Mr. John Nordine, (847) 467-2678

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2003 PHASE I

Novel Polymer Nanocomposite Processing - DOE Contact Charlie Russomanno, (202) 586-7543; ALD NanoSolution, Inc. Contact Dr. Karen J. Buechler, (720) 840-1610

Nanostructured Polymeric Heterogeneous Catalyst for Industrial Applications - DOE Contact Charlie Russomanno, (202) 586-7543; TDA Research, Inc. Contact Mr. John Wright, (303) 940-2300

Development of Silicon Nanocrystals as High Energy White Phosphors - DOE Contact James Brodrick, (202) 586-1856; InnovaLight, Inc. Contact Mr. Paul Thurk, (512) 795-5835

Novel Approach Toward High Performance Energetic Rays Detection - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Lutronics Inc. Contact Dr. Yalin Lu, (978) 387-9685

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2003 PHASE II (FIRST YEAR)

Waveshifters and Scintillators for Ionizing Radiation Detection - DOE Contact Michael P. Procario, (301) 903-2890; Ludlum Measurements, Inc. Contact Mr. Donald Ludlum, (915) 235-5494

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2003 PHASE II (SECOND YEAR)

Virtual-Impact Particle Sizing for Precursor Powders of Nb_3Sn and Bi-2212 Superconductors - DOE Contact Bruce Strauss, (301) 903-3705; Accelerator Technology Corporation Contact Peter McIntyre, (979) 255-5531

Innovative Processing Methods for Superconducting Materials - DOE Contact Bruce Strauss, (301) 903-3705; Alabama Cryogenic Engineering, Inc. Contact Ms. Mary T. Hendricks, (256) 536-8629

Oxide Dispersed Nanofluids for Next Generation Heat Transfer Fluids - DOE Contact Glenn Strahs, (202) 586-2305; Nanopowder Enterprises, Inc. Contact Dr. Gary S. Tompa, (732) 885-1088

Plasma Spraying of $Nd_2Fe_{12}B$ Permanent Magnet Materials - DOE Contact Sam Bader, (630) 252-4960; Aps Material, Inc. Contact Mr. Joseph Cheng, (937) 278-6547

INSTRUMENTATION AND FACILITIES

FY 2003 PHASE I

Using Electrical Resistivity Techniques to Monitor the Long-Term Health of Sub-Surface Reactive Barriers – DOE Contact Justine Alchowiak, (202) 586-4629; Vista Engineering Technologies, LLC Contact Mr. Phillip C. Ohl (509) 737-1377

OFFICE OF FUSION ENERGY SCIENCES

The mission of the Office of Fusion Energy Sciences (OFES) is to advance plasma science, fusion science, and fusion technology—the knowledge base needed for an economically and environmentally attractive fusion energy source. Fusion materials research is a key element of the longer-term OFES mission, focusing on the effects on materials properties and performance from exposure to the radiation, energetic particle, thermal, and chemical environments anticipated in the chambers of fusion experiments and energy systeMs.

The unique requirements on materials for fusion applications are dominated by the intense energetic neutron environment characteristic of the deuterium-tritium fusion reaction. Materials in the fusion chamber must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, "low activation" materials must be selected with activation products that neither decay too rapidly (affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components).

Structural materials research focuses on issues of microstructural stability, fracture and deformation mechanics, and the evolution of physical and mechanical properties. This research provides a link between fusion and other materials science communities and contributes in niche areas toward grand challenges in general fields of materials science. Growth in the theory, modeling, and simulation elements of this research are providing for leveraging of advances in nano-technology and computational materials science research.

Non-structural materials research focuses on plasma-facing materials that protect structural materials from intense heat and particle fluxes and extract surface heat deposited by plasmas without rapid deterioration and or emitting levels of impurities that could degrade plasma performance.

Fusion materials research is conducted with a high degree of international cooperation. Bilateral agreements with Japan enhance the ability of each party to mount fission reactor irradiation experiments. Agreements under the International Energy Agency provides for the exchange of information and the coordination of fusion materials programs in the US, Japan, Europe, Russia, and China. The DOE Contact is S. Berk, (301)-903-4171.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

228. **VANADIUM ALLOY AND INSULATING COATING RESEARCH**
$1,500,000
DOE Contact: S. Berk (301) 903-4171
ORNL Contact: S. Zinkle (865) 576-7220

Research is aimed at vanadium-based alloys for structural application in the chambers of fusion systeMs. The goals of the research, which focuses on the V-Cr-Ti system, are to identify promising candidate compositions, determine the properties of candidate alloys, and evaluate the response to irradiation conditions for anticipated fusion system operation. Critical issues include irradiation embrittlement (loss of fracture toughness), high-temperature creep, impurity corrosion, and joining. Compatibility studies are conducted between vanadium alloys and other candidate fusion materials, focusing on the effects of exposure to candidate coolants. Research is also conducted on electrically insulating coatings for elevated temperature environments. This work identifies promising candidate coating systems, develops coating technology, and conducts the experiments to demonstrate stability and self-repair needed for fusion applications. Work on vanadium alloys involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Vanadium, Compatibility, Lithium, Irradiation Effects, Alloy, Coatings

229. **THEORY AND MODELING**
$1,700,000
DOE Contact: S. Berk (301) 903-4171
UCLA Contact: Nasr Ghoniem (310) 825-4866

Models and computer simulation, validated with experimental data, are combined to extend the understanding of the primary damage processes from irradiation effects. Research is directed at developing a fundamental understanding of both the basic damage process and microstructural evolution that takes place in a material during neutron irradiation.. The goal is to establish models and methods that are able to extrapolate from the available data base to predict the behavior of structural components in fusion systeMs. Special attention is given to the energy range appropriate for the 14 MeV neutrons. Multiscale modeling applies results to evaluate the effects on properties of materials, especially the interactions of the irradiation produced defects with the flow dislocations during deformation processes. Investigations are conducted on (a) the limits of strength and toughness of materials based on dislocation propagation and interactions with crystalline matrix obstacles (b) changes to thermal and electrical conductivity in materials based on electron and photon transport and scattering at the atomic level (c) plastic instabilities and fracture processes in materials irradiated under projected fusion conditions, and (d) effects of the many materials, irradiation, and mechanical loading parameters on flow and fracture processes to establish understanding of controlling mechanisMs. Techniques include atomistic computer simulation, atomic cluster modeling, Monte Carlo analysis, 3-D dislocation dynamics, and flow and fracture models. Research includes materials and conditions relevant to inertial fusion systems as well as magnetic systeMs.

Keywords: Modeling, Simulation, Irradiation Effects

230. **FERRITIC/MARTENSITIC STEEL RESEARCH**
$2,300,000
DOE Contact: S. Berk (301) 903-4171
ORNL Contacts: S. J. Zinkle (865) 576-7220

Research is aimed at iron-based alloys for structural application in the chambers of fusion systeMs. The goals of the research, which focuses on advanced ferritic/martensitic steel systems, are to identify promising candidate compositions, determine the properties of leading candidate alloys, and evaluate the response to irradiation conditions that simulate anticipated fusion system operation. Critical issues include irradiation embrittlement (focusing on DBTT transition shifts and loss of fracture toughness) and high temperature creep. Innovative nanocomposited steels are being explored for higher temperature applications that currently available ferritic steels. Work on this material class involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Steels, Irradiation Effects

231. **SiC/SiC COMPOSITES RESEARCH**
$1,500,000
DOE Contact: S. Berk (301) 903-4171
PNNL Contacts: R. J. Kurtz (509) 373-7515

Research is aimed at SiC/SiC composites for structural application in the chambers of fusion systeMs. This research is directed at furthering the understanding of the effects of irradiation on the SiC/SiC composite systems as the basis for developing superior composite materials for fusion structural applications. The focus of the work is on the evaluation of improved fibers and alternative interface layer materials. Critical issues include irradiation-induced reduction in thermal conductivity, leak-tightness, joining, and helium effects. Work on this material class involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Silicon Carbide, Composites, Irradiation Effects

232. **PLASMA FACING MATERIALS RESEARCH**
$2,000,000
DOE Contact: S. Berk (301) 903-4171
SNL Contact: M. Ulrickson (505) 845-3020

Plasma-facing materials must withstand high heat and particle fluxes from normal operation of fusion plasmas, survive intense surface energies from abnormal fusion plasma operation, such as plasma disruptions, withstand radiation damage by energetic neutrons, achieve sufficient lifetimes and reliability to minimise replacement frequency, and provide for reduced neutron activation to minimize decay heat and radioactive waste burdens. Research activities include improved techniques for joining beryllium or tungsten to copper alloys, development of joining techniques for refractory metals (e.g., W, Mo, Nb, V), development of enhancement schemes for helium cooling or liquid lithium cooling of refractory alloys, and thermal fatigue testing of tungsten and other refractory materials. The joining techniques being investigated include diffusion bonding, hot-isostatic pressing, furnace brazing and inertial welding. Tritium retention and permeation measurements are conducted in the Tritium Plasma Experiment and the PISCES plasma simulator facility. Refractory material work is centered on developing high temperature helium gas cooled or liquid metal cooled heat sinks for plasma facing components. The thermal fatigue testing and heat removal capability measurements are carried out on electron beam test systeMs.

Keywords: Plasma-Facing Materials, Refractory Metals

OFFICE OF BIOLOGICAL & ENVIRONMENTAL RESEARCH

The Biological and Environmental Research (BER) program develops the knowledge needed to identify, understand, anticipate, and mitigate the long-term health and environmental consequences of energy production, development, and use. As the founder of the Human Genome Project, BER continues to play a major role in biotechnology research and also invests in basic research on global climate change and environmental remediation.

The projects listed in this report are managed under the Environmental Management Research Program (EMSP). Basic research under the EMSP contributes to environmental management activities that decrease risk to the public and workers, provide opportunities for major cost reductions, reduce time required to achieve the Department’s environmental management goals, and, in general, address problems that are considered intractable without new knowledge. The entire EMSP portfolio can be viewed on the World Wide Web by accessing the EMSP home page at http://emsp.em.doe.gov. The EMSP program was transferred to the Office of Science in FY 2003. The current EMSP Director is Roland F. Hirsch, (301) 903-9009.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

233. **RADIATION EFFECTS ON SORPTION AND MOBILIZATION OF RADIONUCLIDES DURING TRANSPORT THROUGH THE GEOSPHERE**
$60,000
DOE Contact: Roland F. Hirsch (301) 903-9009
University of Michigan Contacts: Lu-Min Wang, (313) 647-8530

Site restoration activities at DOE facilities and the permanent disposal of nuclear waste inevitably involve understanding the behavior of materials in a radiation field. Radionuclide decay and associated radiation effects lead to physical and chemical changes in important properties (e.g., sorption and cation exchange capacity). During the past three years, radiation effects in selected near-field materials have been evaluated in accelerated laboratory experiments utilizing energetic electrons and ions and *in situ* transmission electron microscopy (TEM). Zeolites and layered silicates were found to be highly susceptible to irradiation-induced solid-state amorphization. The critical doses for complete amorphization of these phases are as low as <0.1 displacement per atom (dpa) or 108 GY in ionization energy deposition (i.e., the dose for a zeolite with 10 wt.% loading of ^{137}Cs in 400 years). Even partial amorphization will cause a dramatic reduction (up to 95%) in ion-exchange and sorption/desorption capacities for radionuclides, such as Cs and Sr. Because the near-field or chemical processing materials, e.g., zeolites or crystalline silicotitanate (CST), will receive a substantial radiation dose after they have incorporated radionuclides, the results suggest that radiation may, in some cases, retard the release of sorbed or ion-exchanged radionuclides. These results have a direct bearing on repository performance assessments (e.g., the extent to which zeolites can retard the release of radionuclides) and on the technologies used to process high-level liquid waste (e.g., separation of 137Cs from HLW using CST at the Savannah River Site).

Radionuclides to be studied include Cs, Sr, U, and Se, which are important because: 1)they represent a range of sorptive behavior that should bracket the behavior of most other radionuclides (except ^{99}Tc) and 2) they are considered to make important contributions to total radiation exposures, as illustrated in the recent Total Systems Performance Assessment-Viability Assessment of the proposed repository at Yucca Mountain. Selected clay and zeolite samples will be irradiated with high energy electrons, high energy ions and neutrons to simulate the radiation
effects from a variety of radioactive decay processes at a much accelerated rate using a unique combination of irradiation facilities available at the University of Michigan (the Ford Nuclear Reactor and the Michigan Ion Beam Laboratory). Ion exchange/sorption experiments will be conducted on samples irradiated to various doses to determine the impact of the radiation effects on the sorption capacity and retention of radionuclides. Novel ion implantation and surface analysis techniques, e.g., atomic force microscopy and Z-contrast high resolution scanning transmission electron microscopy (STEM), will be used to identify atomic-scale effects of radiation damage associated with single or small clusters of radionuclides sorbed onto mineral surfaces.

Keywords: Radiation Effects, Near-Field, Geologic Repository

234. **IRON PHOSPHATE GLASSES: AN ALTERNATIVE FOR VITRIFYING CERTAIN NUCLEAR WASTES**
$79,000
DOE Contact: Roland F. Hirsch (301) 903-9009
University of Missouri-Rolla Contact: Delbert E. Day (573) 341-4354

Borosilicate glass is the only material currently approved and being used to vitrify high level nuclear waste. Unfortunately, many high level nuclear waste feeds in the U.S. contain components which are chemically incompatible with borosilicate glasses. Current plans call for vitrifying even these problematic waste feeds in borosilicate glasses after the original waste feed has been pre-processed and/or diluted to compensate for the incompatibility. However, these pre-treatment processes, as well as the larger waste volumes resulting from dilution, will add billions of dollars to the DOE's cost of cleaning up the former nuclear weapons production facilities. Such additional costs may be avoided by developing a small number of alternative waste glasses which are suitable for vitrifying those specific waste feeds that are incompatible with borosilicate glasses.

A low cost and technically effective alternative waste form based on a new family of iron-phosphate glasses which appear to be well suited for many waste feeds, especially those which are incompatible with borosilicate glasses, has recently been developed. However, the scientific and technical knowledge base that is needed to vitrify nuclear waste in iron phosphate glasses on a production scale is currently lacking. In addition, the high priority wastes that are likely to cause problems in borosilicate melts need to be identified and property data need to be acquired for iron phosphate wasteforms made from these wastes. This research is addressing these needs, using techniques such as EXAFS, XANES, XPS, X-ray and neutron diffraction, IR, SEM, Mössbauer spectroscopy and DTA/DSC to obtain the information needed to demonstrate that iron phosphate glasses can be used to vitrify those nuclear wastes which are poorly suted for borosilicate glasses.

Keywords: Iron Phosphate Glasses, Vitrification, Nuclear Waste

235. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$206,000
DOE Contact: Roland F. Hirsch (301) 903-9009
PNNL Contact: William J. Weber (509) 376-3644

The objective of this project is to develop a fundamental understanding of radiation effects in glass and ceramics, as well as the influence of radiation effects on aqueous dissolution kinetics. This study will provide the underpinning science to develop improved glass and ceramic waste forms for the immobilization and disposition of high-level tank waste, excess plutonium, plutonium residues and scrap, surplus weapons plutonium, other actinides, and other nuclear waste streaMs. Furthermore, this study will develop predictive models for the performance of nuclear waste forms and stabilized nuclear materials. The research focuses on the effects of alpha and beta decay on defect production, defect interactions, diffusion, solid-state phase transformations, and gas accumulation, and dissolution kinetics. Plutonium incorporation, gamma irradiation, ion-beam irradiation, and electron beam irradiation are used to simulate the effects of alpha decay and beta decay on relevant glasses and ceramics in experimental studies. Computer simulation methods are used to provide an atomic-level interpretation of experimental data, calculate important fundamental parameters, and provide multi-scale computational capabilities over different length (atomic to macroscopic) and time (picoseconds to millenia) scales.

Keywords: Glass, Ceramics, Radiation Effects

236. **NEW METAL NIOBATE AND SILICOTITANATE ION EXCHANGERS: DEVELOPMENT AND CHARACTERIZATION**
$310,000
DOE Contact: Roland F. Hirsch (301) 903-9009
PNL Contact: Yali Su (509) 376-5290
SNL Contact: Tina Nenoff (505) 844-0340
UC Davis Contact: Alexandra Navrotsky (916) 752-3292

Previous research by this group provided preliminary data of a novel class of niobate-based molecular sieves (Na/Nb/M/O, M=transition metals) that show exceptionally high selectivity for divalent cations under extreme conditions (acid solutions, competing cations) and novel silicotitanate phases that are also selective for divalent cations. Furthermore, these materials are easily converted by a high-temperature *in situ* heat treatment into a refractory ceramic waste form with low cation leachability. The new niobate-based waste form is a perovskite phase, which is also a major component of Synroc, a titanate ceramic waste form used for sequestration of high-level wastes (HLW) from reprocessed, spent nuclear fuel. These new niobate ion exchangers also showed orders of magnitude better selectivity for Sr^{2+} under acid conditions than any other material.

The goal of this project is to provide DOE with alternative materials that can exceed the performance of monosodium titanate (MST) for strontium and actinide removal at the Savannah River Site (SRS), remove strontium from acidic waste at Idaho National Engineering and Environmental Laboratory (INEEL), and sequester divalent cations from contaminated groundwater and soil plume. The research team will focus on three tasks that will provide both the basic research necessary for the development of highly selective ion exchange materials and also materials for short-term deployment within the DOE complex:
1) structure/property relationships of a novel class of niobate based molecular sieves (Na/Nb/M/O, M=transition metals), which show exceptionally high selectivity for divalent cations under extreme conditions (acid solutions, competing cations); 2) the role of ion exchanger structure change (both niobates and silicotitanates) on the exchange capacity (for elements such as strontium and actinide-surrogates), whichresult from exposure to DOE complex waste simulants; 3) thermodynamic stability of metal niobates and silicotitanate ionexchangers.

Keywords: Niobate, Silicotitanate, Ion Exchanger

237. **PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW**
$240,000
DOE Contact: Roland F. Hirsch (301) 903-9009
Pennsylvania State University Contact: Michael Grutzeck (814) 863-2779
Savannah River Technology Center Contact: Carol M. Jantzen (803) 725-2374

Natural and synthetic zeolites are extremely versatile materials. They can adsorb a variety of liquids and gases, and also take part in cation exchange reactions. Zeolites are easy to make, they can be synthesized from a wide variety of natural and man made materials. One such combination is metakaolinite and sodium hydroxide solution. The objective of this research is to adapt this well known reaction for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites.

It has been established that a mixture of calcined equivalent ICPP waste (sodium aluminate/hydroxide solution containing 3:1 Na:Al) and fly ash and/or metakaolinite can be cured at various temperatures to produce a monolith containing Zeolite A (80°C) or Na-P1 plus hydroxysodalite (130°C) dispersed in an alkali aluminosilicate hydrate matrix. The zeolitization process is a simple one and as such could be a viable alternative for fixation of low activity waste (LAW) salts and calcines. Dissolution tests have shown these materials to have superior retention for alkali, alkaline earth and heavy metal ions.

The technology for synthesizing zeolites is well documented for pure starting materials, but relatively little is known about the process if metakaolinite is mixed with a complex mixture of oxides containing nearly every element in the periodic table. The purpose of the proposed work is to develop a clearer understanding of the advantages and limitations of producing a zeolite-containing waste form from calcined radioactive waste, i.e. the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on their performance. To accomplish this, two waste forms representative of solutions in storage at the Hanford and Savannah River sites will be simulated. Because nitrate is detrimental to the process, the LAW will be calcined at various temperatures (w/wo sugar) to maximize the reactivity of the resultant mix of oxide phases while minimizing the loss of volatiles. The oxides will be mixed with varying amounts and types of metakaolinite, small amounts of other chemicals (alkali hydroxides and/or carbonates, zeolite seeds, templating agents) and enough water to make a paste. The paste will then be cured (in-can) at a variety of temperatures (80°-100°C). Once reaction rates for the process are established, MAS NMR and TEM will be used to study the atomic-level structure of the solids. X-ray diffraction will be used to examine the degree of crystallinity of the waste forMs. An environmental SEM will be used to track the development of microstructure in real time. An electron microprobe will be used to analyze the phases in the waste form. Attempts will be made to relate changes in phase chemistry and microstructure to distribution coefficients and dissolution data. Compressive and bending strength tests will be used to determine mechanical behavior and standard leach tests will be used to determine the potential consequences of cation exchange reactions. Since simulated waste is not an adequate predictor, a major portion of the proposed work will be carried out at the Savannah River Technology Center, using actual LAW samples obtained from the Savannah River site.

Keywords: Zeolites, Radioactive Waste

238. **INVESTIGATING ULTRASONIC DIFFRACTION GRATING SPECTROSCOPY AND REFLECTION TECHNIQUES FOR CHARACTERIZING SLURRY PROPERTIES**
$235,000
DOE Contact: Roland F. Hirsch (301) 903-9009
Pacific Northwest National Laboratory Contact: Margaret S. Greenwood (509) 375-6801
University of Washington Contact: Lloyd W. Burgess (206) 543-0579

The U.S. Department of Energy (DOE) has millions of gallons of radioactive liquid and sludge wastes that must be retrieved from underground storage tanks. This waste, in the form of slurries, must be transferred and processed to a final form, such as glass logs. On-line instrumentation to measure the properties of these slurries in real-time during transport is needed in order to prevent plugging and reduce excessive dilution. This project is a collaborative effort between Pacific Northwest National Laboratory (PNNL) and the University of Washington to develop a completely new method for using ultrasonics to measure the particle size and viscosity of a slurry. The concepts are based on work in optics on grating-light-reflection spectroscopy (GLRS) at the University of Washington and some preliminary work on ultrasonic diffraction grating spectroscopy (UDGS) that has already been carried out at PNNL. The project objective is to extend the GLRS theory for optics to ultrasonics, and to demonstrate its capabilities of UDGS. The viscosity of a slurry is measured by using the multiple reflections of a shear wave at the slurry-solid interface. This new ultrasonic method could result in an instrument that would be simple, rugged, and very small, allowing it to be implemented as part of a pipeline wall at facilities across the DOE complex.

Keywords: Diffraction Grating, Spectroscopy, Ultrasonic, Slurry, Viscosity, Particle Size

239. **CHEMISTRY OF ACTINIDES IN MOLTEN GLASSES AND ITS CORRELATION TO STRUCTURAL PERFORMANCE OF SOLID GLASSES: FILLING THE KNOWLEDGE GAP**
$100,000
DOE Contact: Roland F. Hirsch (301) 903-9009
Oak Ridge National Laboratory Contact: Sheng Dai (865) 576-7307
Savannah River Technology Center Contact: Ray F. Schumacher (803) 725-5991

Chemical processes occurring in molten glasses are key elements in determining efficient immobilization and the long term stability of glasses. The underlying goal of this research is to make use of high-temperature spectroscopic techniques to increase our fundamental understanding of the vitrification process, specifically the relationship between the chemistry of molten glasses and the structural features of final solid glasses. The fundamental knowledge gained in this study will fill a crucial knowledge gap concerning chemistry of actinides in molten glasses and have a broad impact on the design and construction of advanced vitrification processes. High temperature UV/Visible and near-IR spectral data will be used to investigate the solubility of actinide species in various molten glasses as a function of the composition and temperature. These data will be used to develop a new “optical basicity” scale for actinide stability and speciation in oxide glasses in analogy to the common pH scale used to define the acid-base properties of aqueous systeMs. Fluorescence lifetime distribution methods, fluorescence line-narrowing spectroscopy and X-ray absorption spectroscopy (XAS) will provide information on the local environment of the actinides while EPR and x-ray absorption edge positions will be used to define the oxidation states of actinide species in glasses. The combination of the optical basicity scale and structural information from fluorescence and XAS investigations, will be used to produce a detailed description of the identities and behavior of actinide species in silicate-based glasses. This stability model will be correlated to actinide leaching behavior for a glass matrix and offers a simple but powerful set of spectral “fingerprints” to predict the behavior of actinide species when immobilized in a glass.

Keywords: Molten Glasses, Spectroscopy, X-ray Absorption, Actinides

240. **STABILITY OF HIGH LEVEL RADIOACTIVE WASTE FORMS**
$190,000
DOE Contact: Roland F. Hirsch (301) 903-9009
Oak Ridge National Laboratory Contact:
Theodore M. Besmann (865) 574-6852
Pacific Northwest National Laboratory Contact:
John D. Vienna (509) 372-2807

High-level waste (HLW) glass compositions, processing schemes, limits on waste loading, and corrosion/dissolution release models are dependent on an accurate knowledge of liquidus temperatures and thermochemical values. Unfortunately, existing models for the liquidus are empirically-based, depending on extrapolations of experimental information. In addition, present models of leaching behavior of glass waste forms use simplistic assumptions of the thermochemistry or experimentally measured values obtained under non-realistic conditions. There is thus a critical need for both more accurate and more widely applicable models for HLW glass behavior. In a previous project significant progress was made in modeling HLW glass. Borosilicate glass was accurately represented along with the additional FeO-Fe_2O_3, Li_2O, K_2O, MgO, and CaO components. Nepheline precipitation, an issue in Hanford HLW formulations, was modeled and shown to be predictive. The objective of this effort is to continue the development of a basic understanding of the phase equilibria and solid solution of HLW glasses, incorporating other critical waste constituents including, S, Cr, F, P, actinides and rare earths. With regard to a fundamental understanding of solution oxides, there should be added insights on defect chemistry, interstitial behavior, clustering, and the energetics of metal oxide solutes.

Keywords: High-Level Waste, Glass, Phase Equilibria

241. **PHYSICAL CHARACTERIZATION OF SOLID-LIQUID SLURRIES AT HIGH WEIGHT FRACTIONS UTILIZING OPTICAL AND ULTRASONIC METHODS**
$240,000
DOE Contact: Roland F. Hirsch (301) 903-9009
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Savannah River Technology Center Contact:
Carol M. Jantzen (803) 725-2374

Liquid sodium-bearing waste (SBW) can be calcined and solidified using metakaolinite and a limited amount of water. The processing does not require expensive specialized equipment or exotic materials but rather it can be done using conventional cement and/or concrete mixing equipment. The final product is cured at relatively low temperatures producing a dense ceramic-like material (hydroceramic) with strength in the 300-400 psi range and leach rates comparable to glass waste forms with similar waste loading. This product is stable in realistic geologic settings due to the *in situ* growth of zeolites. Data from a previous project have shown that hydroceramics could well be a viable alternative for fixation of low activity sodium-bearing waste. The objective of this continuation study is to further adapt this technology for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites. This work is aimed at developing a clearer understanding of the advantages and limitations of producing a zeolite-containing hydroceramic from the low activity SBW at these sites, i.e., the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on the performance of the waste form. In addition, the processing method will be further refined to increase waste loading in the hydroceramics, with the objective of making the calcine fit the zeolitization process as well as possible. It is anticipated that by tailoring the calcination process, it will be possible to encapsulate many more radionuclides without sacrificing the performance of the waste form, thereby creating a better hydroceramic waste form.

Keywords: Hydroceramic, Zeolites, Sodium-Bearing Waste, Calcination

242. **ASSESSING THE STATE AND DISTRIBUTION OF RADIONUCLIDE CONTAMINATION IN CONCRETE: AN EXPERIMENTAL AND MODELING STUDY OF THE DYNAMICS OF CONTAMINATION**
$300,000
DOE Contact: Roland F. Hirsch (301) 903-9009
Lawrence Livermore National Laboratory Contact: Brian Viani (925) 423-2001

There are hundreds of cement structures in the DOE complex that are contaminated by radionuclides and otherchemicals. A fundamental understanding of the factors governing contaminant interactions in concrete is necessary in order to evaluate and model contaminant transport and develop more efficient methods for R&D efforts. The goal of this research is to enhance our understanding of how radionuclides bind to concrete and to develop a more accurate predictive capability which will allow various decontamination approaches to be evaluated. This will be accomplished through a combination of laboratory-based experiments on radionuclide interactions with cementitious materials, along with state-of-the-art materials characterization and transport modeling techniques. Transport studies including flow-through and batch sorption tests will be initiated using the radionuclides Cs, Tc, U, and Pu and ordinary Portland cement with or without aggregates. In addition to standard radioanalytical and microscopic methods, X-ray absorption spectroscopy will be used to provide detailed, element-specific information on radionuclide speciation, including distribution, redox activity, and aging effects. Results from these experiments will be compared to characterization of actual aged concrete cores from contaminated DOE facilities. Transport modeling simulations will use the chemical parameters determined from the lab-based experiments and the materials characterization tasks to predict the depth of contaminant penetration and its chemical form and association in the concrete. Our simulations explicitly account for fracture flow and mineralogical heterogeneity and will be used to predict the effect of fractures and aggregate on the resulting radionuclide distribution. The team assembled here has extensive background and experience in studying radionuclide interactions with cementitious materials.

Keywords: Radionuclides, Contamination, Concrete, Modeling, Transport

243. **UNDERGROUND CORROSION AFTER 32 YEARS:A STUDY OF FATE AND TRANSPORT**
$260,000
DOE Contact: Roland F. Hirsch (301) 903-9009
Idaho National Engineering and Environmental Laboratory Contact: Kay Adler Flitton (208) 526-0525

In 1970, the National Institute of Standards and Technology (NIST) implemented the most ambitious and comprehensive long-term corrosion behavior test to date for stainless steels in soil environments. Thirty-three years have passed since scientists buried 6,324 specimens from stainless steel types, specialty alloys, composite configurations, and multiple material forms and treatment conditions at six distinctive soil-type sites throughout the country. Today, there are more than 190 specimens per site, exceeding a total of 1000 specimens that remain undisturbed, a buried treasure of subsurface scientific data. The objective of this research project is to complete the NIST corrosion study and thoroughly examine the soil and environment surrounding the specimens. The project takes an interdisciplinary research approach that will correlate the complicated interrelationships among metal integrity, corrosion rates, corrosion mechanisms, soil properties, soil microbiology, plant and animal interaction with corrosion products, and fate and transport of metallic ions. The results will provide much needed data on corrosion rates, underground material degradation, and the behavior of corrosion products in the near-field vadose zone. The data will improve the ability to predict the fate and transport of chemical and radiological contaminants at sites throughout the DOE complex. This research also directly applies to environmental management operational corrosion issues, and long-term stewardship scientific needs for understanding the behavior of waste forms and their near-field contaminant transport.

Keywords: Metals, Corrosion, Transport, Contaminants

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

	FY 2003
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY - GRAND TOTAL	$9,476,000
OFFICE OF SPACE AND DEFENSE POWER SYSTEMS	$6,466,000
SPACE AND NATIONAL SECURITY PROGRAMS	$6,466,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,945,000
Maintain the Capabilities and Facilities to Produce DOP-26 Iridium Alloy Blank and Foil Stock Material, Manufacture Clad Vent Sets, and Manage the Iridium Inventory	1,575,000
Carbon-Bonded Carbon Fiber Insulation Production, Maintenance, Manufacturing Process Development, and Product Characterization	370,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING	$4,521,000
Alloy Development Characterization, Mechanical Property Testing, and Insulation	1,140,000
Heat Source Fabrication Development and Materials Testing for IHS70 Program	500,000
Pu-238 Production Studies	2,881,000
OFFICE OF ADVANCED NUCLEAR RESEARCH	$3,010,000
ADVANCED FUEL CYCLE INITIATIVE	$2,260,000
Radiation Damage Modeling in AFCI Materials	100,000
Lead Alloy Technology	1,660,000
Structural Materials Testing	500,000
NUCLEAR HYDROGEN INITIATIVE	$750,000
Development of Advanced High-Temperature Heat Exchangers	750,000

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

OFFICE OF SPACE AND DEFENSE POWER SYSTEMS

SPACE AND NATIONAL SECURITY PROGRAMS

Programs within the Office of Space and Defense Power Systems include the development and production of radioisotope power systems (RPS) for both space and terrestrial applications and providing technical direction, planning, demonstration, and delivery of space fission power and propulsion systems.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

244. **MAINTAIN THE CAPABILITIES AND FACILITIES TO PRODUCE DOP-26 IRIDIUM ALLOY BLANK AND FOIL STOCK MATERIAL, MANUFACTURE CLAD VENT SETS, AND MANAGE THE IRIDIUM INVENTORY**
$1,575,000
DOE Contact: John Dowicki (301) 903-7729
ORNL Contacts: Jim King (865) 574-4807, Evan Ohriner (865) 574-8519, George Ulrich (865) 576-8497

The DOP-26 Iridium alloy is the fuel clad capsule material for radioisotope heat sources in NASA space power systems. The production capabilities and facilities for producing blank and foil stock material at ORNL was maintained by continuing all production activities to supply limited quantities of blanks and foil for clad vent set (CVS) production maintenance activities. The CVS production activity produces flight quality components for inventory and maintains the production capabilities for future production campaigns. The iridium inventory for DOE is maintained, audited, and reported annually.

During FY 2003, 53 flight quality iridium alloy blanks were produced and removed from storage and transferred to the CVS Production Task. Extensive repair work was performed on the 1200-Ton extrusion press to rebuild valves and other components. Experiments were conducted to develop a method of removing thorium from scrap iridium alloy to prepare it for refining. Ten flight quality CVS's were produced in FY 2003 and shipped to Los Alamos National Laboratory. The Annual Iridium Inventory Report was issued.

Keywords: Iridium Processing, Melting, Extrusion, Clad Vent Sets

245. **CARBON-BONDED CARBON FIBER INSULATION PRODUCTION, MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT, AND PRODUCT CHARACTERIZATION**
$370,000
DOE Contact: John Dowicki (301) 903-7729
ORNL Contacts: Jim King (865) 574-4807 and Glenn Romanoski (865) 574-4838

The CBCF production facilities have been operated in a production maintenance mode since the Cassini campaign to produce flight quality insulators sets. Dedicated facilities for the CBCF production remain in the Carbon Materials Technology Laboratory at ORNL. The impurity content of CBCF insulators produced in FY 2001 and FY 2002 had become an issue with respect to qualifying insulators as flight quality. All aspects of the production process were examined from the starting materials to the various processing steps. The issues were resolved and eight flight quality insulator sleeves and forty disks were produced in FY 2003.

Keywords: Insulation/Thermal, High Temperature Service, Carbon Fibers

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING

246. **ALLOY DEVELOPMENT CHARACTERIZATION, MECHANICAL PROPERTY TESTING, AND INSULATION**
$1,140,000
DOE Contact: John Dowicki (301) 903-7729
ORNL Contacts: Jim King (865) 574-4807 and Easo George (865) 574-5085, Robert Swindeman (865) 574-5108

The activity provides the materials characterization, mechanical property information, and assessment of material behavior in specific applications to support various RPS Program needs. The characterization of iridium alloy DOP-26 has identified the effect of various impurities on the alloy properties and its manufacturing and service reliability. An alternate iridium alloy (DOP-40) containing less thorium and the addition of cerium has been developed and shown to have desirable properties. Mechanical property determinations are made on various alloys after thermal aging to assess their suitability for long-term terrestrial and space missions.
Significant progress was made in several areas during FY 2003. Capsule pressure burst equipment which had been developed for a heat source program was utilized to test weld qualification capsules fabricated at LANL and ANL-W. This testing was successfully completed and a preliminary report was distributed with the results. Creep and creep-rupture testing of Haynes 25 alloy continued and an interim report was issued with the results.

Equipment was prepared to continue the aging of Haynes 25 beyond 12,000 hours. An investigation of the compatibility of Haynes 25 with graphite in a simulated generator environment was initiated and results for exposure times to 4560 hours were obtained and reported. The results showed no embrittlement of the alloy in these tests compared to similar samples aged in vacuum. Thermal aging studies were also continued on Mo-41%Re alloy and tensile test results of these aged specimens showed no deleterious effect on ductility after 2880 hours at temperatures in the range of 500˚ to 700˚C.

Keywords: Iridium Alloy, Compatibility, Thermal Aging

247. **HEAT SOURCE FABRICATION DEVELOPMENT AND MATERIALS TESTING FOR IHS70 PROGRAM**
$500,000
DOE Contact: John Dowicki (301) 903-7729
ORNL Contact: Jim King (865) 574-4807

A radioisotope power system generator is being developed which utilizes iridium clad fuel enclosed in capsules of Ta-10W alloy, molybdenum, and Haynes 230. The Ta-10W capsule is designed to retain helium pressure during the service life. The outer capsule of Haynes 230 protects the refractory alloy from oxidation. ORNL is responsible for producing these capsule components for the new heat source. The iridium capsules will be longer than the standard clad vent set to accommodate a larger fuel pellet. ORNL will conduct testing to produce a mechanical property data base to support the materials selection and design requirements.

Fabrication development was initiated for the various heat source components. A large heat of Ta-10W was procured and received. Haynes 230 alloy and molybdenum was also received. Forming dies and fixtures were designed and fabricated for this project. Forming development was performed for the iridium long clad vent sets in addition to the Ta alloy, Haynes alloy, and molybdenum components. A Ta-10W oxidation study was initiated to determine the effects of oxygen on the tensile ductility of the alloy as a function of temperature. Refurbishment of ultra-high vacuum creep machines was initiated and components were procured for the assembly of an instrumented ultra-high vacuum capsule pressure-burst chamber and a tensile testing machine.

Keywords: Ta-10w Oxidation, Refractory Metals, Mechanical Properties

248. **PU-238 PRODUCTION STUDIES**
$2,881,000
DOE Contact: Wade Carroll (301) 903-3161
ORNL Contact: Bob Wham (865) 576-7783

Target development studies are required to gain a better understanding of the mechanisms of ^{236}Pu and ^{238}Pu production and to support development of target designs. The target development effort is broken into four phases titled dosimeter target, pellet performance target, array target, and prototype target. During FY 2003, two subtasks under target development will be undertaken. The first subtask was a study to determine the effect of radiolysis of water during long-term storage of NpO_2. The second subtask was to continue the post irradiation examination (PIE) of array targets. These tests focused on dissolving the plutonium produced during irradiation in the Idaho National Laboratory Advanced Test Reactor.

Post-irradiation examination of array targets was conducted during FY 2003 to support target design efforts. Several trends that reflected the various target positions were identified. The percentage of neptunium that is converted to plutonium increases with relative power. The ^{238}Pu production, as a percentage of total plutonium, generally decreases with increasing power. These and other results were compiled in a draft report "Post-Irradiation Examination of Array Targets-Part I," ORNL/TM-2003/220. The results of the water sorption experiment on samples prepared at 650 and 800˚C show that NpO_2 is unlikely to absorb significant water under conditions of 60% relative humidity. The results from the gamma radiolysis experiments with samples containing less than 1% moisture showed an overall pressure decrease as the O_2 over the sample was consumed. It was concluded gamma radiolysis will not be significant in the storage of NpO_2.

Keywords: ^{238}Pu Production, Gamma Radiolysis Experiments

OFFICE OF ADVANCED NUCLEAR RESEARCH

ADVANCED FUEL CYCLE INITIATIVE

The mission of the Advanced Fuel Cycle Initiative (AFCI) is to develop proliferation-resistant spent nuclear fuel treatment and transmutation technologies in order to enable a transition from the current once through nuclear fuel cycle to a future sustainable, closed nuclear fuel cycle. The intermediate-term issues associated with spent nuclear fuel, primarily the reduction of the volume and heat generation of material requiring geologic disposal, will be addressed using advanced separations technologies and proliferation-resistant recycle fuels in existing and advanced light water reactors, and possibly gas-cooled reactors if deployed in the near future. A longer-term effort will develop fuel cycle technologies to destroy minor actinides in fast neutron spectrum systems, greatly reducing the long-term radiotoxicity and heat load of high-level waste sent to a geologic repository. This will be accomplished through the development of a transmutation fuel cycle using Generation IV fast reactors.

249. **RADIATION DAMAGE MODELING IN AFCI MATERIALS**
$100,000
DOE Contact: Sue Lesica (301) 903-8755
LANL Contact: Mike Cappiello (505) 665-6408

Through the modeling of the mechanisms of radiation-induced helium production in body centered cubic iron, this research examines the loss of ductility as a function of helium production and displacements per atom (dpa). Also included is the identification of parameters to be experimentally measured to quantify the predictive model, methods to quantify these parameters experimentally and the proposal of experiments.

Keywords: Modeling, Ferritic Steel, Helium Embrittlement

250. **LEAD ALLOY TECHNOLOGY**
$1,660,000
DOE Contact: Sue Lesica (301) 903-8755
LANL Contact: Mike Cappiello (505) 665-6408

Coolant technology is focused on the development of lead-alloy heat-transport system materials and components. The DEvelopment of Lead-alloys Technologies and Applications (DELTA) lead-bismuth test loop at LANL is the primary facility for this research. The loop is being used to perform corrosion, erosion, compatibility, thermal hydraulic, thermodynamic, radiation environment effects and instrumentation tests, with the support of off-line development of sensors, control systems, measurement and impurity removal techniques, and modeling. In addition to U.S. research, the facility is being used for international collaborations investigating lead coolant technologies. Long-term corrosion tests will be performed to systematically assess the performance of materials during the initial stage of oxide formation. Testing and analysis of specimens, component performance over time and under varying conditions, and lifetime limits will be determined. Development and testing of materials with enhanced corrosion resistance through special alloying and surface treatment will take place concurrently. Materials will be screened and assessed for high temperatures and coolant technology needs beyond oxygen control. Heat transfer and thermal hydraulic tests for reactor (e.g., fuel assembly to coolant heat transfer) and spallation target designs will be planned and performed. For the candidate fuel options, compatibility of coolant with fuel cladding and fuels will be investigated. The effects of radiation on corrosion, activation of corrosion products and mitigation strategies, radiation and spallation product influence on coolant chemistry and mitigation strategies will be studied. These effects will first be studied with surrogates and in simulated environments, and later in integral irradiation campaigns.

Keywords: Lead Bismuth, Transmutation

251. **STRUCTURAL MATERIALS TESTING**
$500,000
DOE Contact: Sue Lesica (301) 903-8755
LANL Contact: Mike Cappiello (505) 665-6408

The objective is to qualify structural materials of interest in a high-flux and high-fluence irradiation environment with high-energy particles relevant to fast-spectrum transmutation. This research examines the effect of high energy proton and neutron radiation on the mechanical properties of structural and target materials that could be used in an accelerator driven transmutation system.

Keywords: Transmutation, Irradiation, Structural Materials

NUCLEAR HYDROGEN INITIATIVE

The President's Hydrogen Fuel Initiative is a new research and development effort to reverse America's growing dependence on foreign oil and expand the availability of clean, abundant energy. Hydrogen is produced today on an industrial scale in the petrochemical industry by a process of steam reforming, using natural gas as both source material and heat source. Recent research conducted under the Department's Nuclear Energy Research Initiative (NERI) indicates the possibility of hydrogen production through the thermochemical splitting of water. Nuclear heat, supplied to a hydrogen-producing thermochemical plant through an intermediate heat exchanger, promises high efficiency and avoids the use of carbon fuels. Using very-high-temperature advanced nuclear reactors, such as Generation IV gas-cooled or liquid metal-cooled reactors, nuclear energy can produce hydrogen in very large quantities consistently over long periods of time without emitting greenhouse gases or other harmful air emissions. The Department is also exploring several other processes, including the high-temperature electrolysis of water.

252. **DEVELOPMENT OF ADVANCED HIGH-TEMPERATURE HEAT EXCHANGERS**
$750,000
DOE Contact: Carl Sink (301/903-5131)
UNLV Contact: Tony Hechanova (702-895-1457)

The goal of this project is to develop high-temperature heat exchangers for hydrogen production and electrical energy conversion from advanced nuclear reactors. The challenge lies in developing heat exchangers that can withstand very high temperatures (850°C and above) and highly reactive and corrosive process fluids. The working fluids include sulfuric acid, hydrogen iodide, and steam/water as the cold fluids and helium or molten salt as the hot fluid Candidate materials for the heat exchangers include the following classes: high-temperature nickel-based alloys, high-temperature ferritic steels (particularly oxide dispersion strengthened), and carbon and silicon carbide composites. Research includes general and localized corrosion studies, tensile testing at high temperatures, TEM, SEM and metallographic examination, stress corrosion cracking tests at elevated temperatures and heat transfer phenomena.

Keywords: Heat Transfer, Ferritic Steels, Composites, Corrosion, Molten Salt, Hydrogen Production

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2003
NATIONAL NUCLEAR SECURITY ADMINISTRATION - GRAND TOTAL	$112,368,000
OFFICE OF NAVAL REACTORS	$83,400,000[20]
OFFICE OF DEFENSE PROGRAMS	$28,968,000
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM	$28,968,000
SANDIA NATIONAL LABORATORIES	$17,535,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$7,254,000
Materials Synthesis	1,010,000
Metal Processing Science	1,085,000
LIGA Processing	875,000
Microstructural and Continuum Evolution Modeling of Sintering	246,000
Biocompatible Self-Assembly of Nano-Materials for Bio-MEMS and Insect Reconnaissance	346,000
Understanding Metal Vaporization from Transient High Fluence Laser Irradiation	81,000
Science Based Processing of Field-Structured Composites	96,000
Design, Synthesis, and Characterization of Soft Matter Nanolayer Superlattices	296,000
Photo-control of Nano-Interactions in Microsystems	271,000
Electrochemically Deposited Alloys with Tailored Nanostructures for LIGA Micromachines	336,000
Solution-Based Nanoengineering of Materials	316,000
Assembly and Actuation of Nanomaterials Using Active Biomolecules	485,000
Decomposition of Contaminants Using Photochemically Active Nanoparticles	396,000
Thermally Cleavable Surfactants	296,000
Transition-Metal Catalyzation of Complex-Hydride Absorption/Desorption Reactions	197,000
Assembly of Ordered Electro-Optical and Bioactive Materials and Composites	396,000
Active Photonic Nanostructures	500,000
Study of Polymer Spin-coating for Photollithographic Semiconductors in Near Zero Gravity Environment	26,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$6,979,000
Materials Performance	900,000
High Pressure and Shock Physics	250,000
Aging of Organic Materials	1,100,000
Corrosion Science and Metal Degradation	1,043,000
Reliability in Microsystem Materials	1,530,000
Nanomechanics	250,000
Magnetic-field Effects on Vacuum-Arc Plasmas	221,000
First-principles Determination of Dislocation Properties	166,000
Dynamics of Metal/ceramic Interfaces	156,000
In-situ Characterization of Soft Solution Processes for Nanoscale Growth	96,000
Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques	156,000
Exploration of New Multivariate Spectral Calibration Algorithms	148,000

[20]This excludes $52.8 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

NATIONAL NUCLEAR SECURITY ADMINISTRATION (continued)

	FY 2003
OFFICE OF DEFENSE PROGRAMS (continued)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (continued)	
SANDIA NATIONAL LABORATORIES (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
Nanostructured Materials for Directed Transport of Excitation Energy	296,000
The Effects of Varying Humidity on Copper Sulfide Film Formation	196,000
Quantification of Environments and Surfaces Within Micro-packages	371,000
Fundamental Mechanisms of Mechanical Response for Nanostructured Materials	100,000
MATERIALS STRUCTURE AND COMPOSITION	$462,000
The Basics of Aqueous Nanofluidics: "Interphase" Structure and Surface Forces	296,000
Modeling Local Chemistry in the Presence of Collective Phenomena	166,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,450,000
Assuring Ultra-clean Environments in Micro-system Packages: Irreversible and Reversible Getters	361,000
Mechanics and Tribology of Mems Materials	266,000
LIGA Microsystems Aging: Evaluation and Mitigation	356,000
Advanced Packaging/joining Technology for Microsystems	321,000
Magnetostrictive Elastomers for Actuators and Sensors	146,000
INSTRUMENTATION AND FACILITIES	$1,390,000
Advanced Analytical Technology Project	990,000
Information Extraction	400,000
LAWRENCE LIVERMORE NATIONAL LABORATORY	$11,433,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$8,500,000
Engineered Nanostructure Laminates	8,500,000
INSTRUMENTATION AND FACILITIES	$2,933,000
AFM Investigations of Biomineralization	113,000
Polyimide Coating Technology for ICF Targets	1,300,000
Beryllium Ablator Coatings for NIF Targets	500,000
Using Dip-Pen Nanolithography to Order Proteins and Colloids at Surfaces	420,000
Plasma Polymer Coating Technology for ICF Targets	600,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION

OFFICE OF NAVAL REACTORS

The Deputy Administrator for Naval Reactors within the National Nuclear Security Administration is responsible for conducting requirements under Section 309(a) of the Department of Energy Organization Act which assigns civilian power reactor programs and all DOE naval nuclear propulsion functions. Executive Order 12344, as set forth in Public Law 106-65, stipulates responsibilities and authority of the Naval Nuclear Propulsion Program, of which the Deputy Administrator for Naval Reactors is a part.

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systeMs. This work includes irradiation testing of reactor fuel, poison, and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property, and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories—Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $136.2 million in FY2003. Approximately $52.8 million represents the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is David I. Curtis, (202) 781-6141.

OFFICE OF DEFENSE PROGRAMS

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

253. **MATERIALS SYNTHESIS**
$1,010,000
DOE Contact: Kimberly Budil
(202) 586-7831
SNL Contacts: Jun Liu (505) 845-9135 and
William R. Even, Jr. (925) 294-3217

This project explores innovative synthesis strategies to create materials to meet specified performance requirements for established and anticipated applications in the enduring stockpile. The overall goal is to establish materials-based options for both passive and active functions critical to the successful execution of both conventional and micro-scale systeMs. Areas of current emphasis include new approaches for removable encapsulants, foams and adhesives, new polymeric materials for MEMS encapsulants, and the control of material structure from the nano- to the meso-scale to provide options for advanced chemical and physical state sensing, filtering and gettering, and photon/radiation manipulation.

Keywords: Encapsulants, Foams, Sensing, Gettering, Polymers

254. **METAL PROCESSING SCIENCE**
$1,085,000
DOE Contact: Kimberly Budil (202) 586-7831
SNL Contact: Mark F. Smith (505) 845-3256 and
Charles H. Cadden (925) 294-3650

The primary focus of this activity is to develop and integrate fundamental understanding, scientific methods, and process modeling to create a knowledge base and enhanced tools for metal manufacturing processes (e.g. welding, active brazing, soldering, thermal spray, melting, and casting) used in the production of non-nuclear components. Activities in this area include the development of innovative new techniques to make in-situ measurements of fundamental properties necessary to better understand process physics and to validate computer process models. We are also studying the effect of hydrogen on metals, because this issue is critical for nuclear weapon systeMs. The control and optimization of microstructure and properties of materials for penetrator casings is being developed. The ultimate goal of this effort is to establish a robust capability for guiding manufacturing process parameter selection and predicting the ultimate performance of manufactured parts.

Keywords: Welding, Brazing, Soldering, Thermal Spray, Hydrogen Effects

255. **LIGA PROCESSING**
$875,000
DOE Contact: Kimberly Budil (202) 586-7831
SNL Contacts: William R. Even (925) 294-3217 and H. Eliot Fang (505) 844-4526

LIGA is a microfabrication technique that uses x-ray lithography and electroplating to create metal microparts. LIGA microparts offer a way to improve manufacturing, decrease tolerances, improve performance, enable new measurement schemes, and reduce the weight and size of weapon components and flight test assemblies. There is a continuing effort in both experimental and computational approaches to understanding and extending LIGA processing in order to enable the widest variety of potential weapon applications with the lowest possible risk. The efforts are aimed at evaluation of the fundamentals of the lithography as well as the electroplating processes, and the relation between the processes and the structure and property of the fabricated parts.

Keywords: Microfabrication, Lithography, Electroplating, Metal, X-ray

256. **MICROSTRUCTURAL AND CONTINUUM EVOLUTION MODELING OF SINTERING**
$246,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Veena Tikare (505) 844-1306

All ceramics and powder metals, including the ceramics components that Sandia uses in critical weapons components such as PZT voltage bars and current stacks, multi-layer ceramic MET's, alumina/molybdenum & alumina cermets, and ZnO varistors, are sintered. Sintering is a critical, possibly the most important, processing step during manufacturing of ceramics. The microstructural evolution, the macroscopic shrinkage, and shape distortions during sintering will control the engineering performance of the resulting ceramic component. Yet, modeling and prediction of sintering behavior is in its infancy, lagging far behind the other manufacturing models, such as powder synthesis and powder compaction models, and behind models that predict engineering properties and reliability. This proposal is to develop a set of computational tools that will enable us to understand, predict, and control microstructural evolution and macroscopic dimensional changes during sintering. Previous research efforts on sintering modeling have failed because they treat some limited aspect of sintering, either on the microstructural or macroscopic continuum scale. Microstructural models treat the evolution of two or three powder particles during sintering to give detailed information about particle shapes and densification rates. However, they fail to treat a macroscopic sintering piece—the shape change, density distribution, stress formation, etc. Continuum models apply continuum deformation mechanics to the sintering body to predict shrinkage and component shape change. However, the deformation equations are poorly understood and not directly linked to real material systems, so application of continuum sintering models to real materials has had limited success. We propose a novel modeling method that can treat the microstructural evolution of thousands of powder particles during sintering and integrate the results into continuum models to predict the overall shrinkage and shape distortions in a sintering component. An equally important result of this work will be a fundamental advancement in the understanding of sintering science.

Keywords: Sintering, Ceramic Manufacturing, Microstructural Evolution, Manufacturing Models

257. **BIOCOMPATIBLE SELF-ASSEMBLY OF NANO-MATERIALS FOR BIO-MEMS AND INSECT RECONNAISSANCE**
$346,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: C. Jeffrey Brinker (505) 272-7627

Cell-based sensors have the potential to integrate, within a very small volume, recognition, amplification, and transduction properties. Unfortunately most cell-based sensor designs require external fluidic systems and electronics to ensure cell viability and addressability, making them impractical as miniaturized sensor platforMs. The overall goal of our project is the development of biocompatible self-assembly procedures enabling the immobilization of genetically engineered cells in a compact, self-sustaining, remotely addressable sensor platform useful for covert insect reconnaissance missions. Key to this concept is patterned cell incorporation in a robust, biocompatible, host that maintains cell viability and accessibility while enabling signal transduction and transmittal. Bulk silica matrices formed by 'classical' sol-gel processing have been used for cell entrapment, but alcohol solvents and broad pore size distributions limit cell viability and accessibility. Furthermore, bulk gels are difficult to integrate into devices like MEMs. Our approach uses evaporation induced self-assembly (EISA) to immobilize cells within periodic silica nanostructures, characterized by unimodal pore sizes and pore connectivity, that can be patterned using robo-writing or ink-jet printing. Since surfactants typically used to direct silica self-assembly are bio-incompatible, this project has devised completely new biocompatible self-assembly approaches to enable both incorporation of whole cells into MEMS architectures and the writing of functional bioactive devices in general. The advantages of biocompatible self-assembly are two-fold. First the templated pores are all the same size. These hydrophilic monosized pore networks will spontaneously fill with water to create a kinetically stable aqueous environment without an auxiliary fluidic system. Second, EISA proceeds in complex mixtures and can direct the formation of nanocomposites so we can immobilize cells in fluidic contact with nanostructured hydrogels that provide a reservoir of buffer and nutrients to sustain viability for times exceeding one week. Through genetic modification, cell-based sensors can be developed for specific CW, BW or explosive threats.

Keywords: Nanostructure, Self Assembly, MEMS, Ink-Jet Printing, Sensors

258. **UNDERSTANDING METAL VAPORIZATION FROM TRANSIENT HIGH FLUENCE LASER IRRADIATION**
$81,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Phillip W. Fuerschbach (505) 845-8877

Laser spot welding is widely used for precision joining of nuclear weapon components and other high reliability devices. The production of metal vapor as a consequence of high intensity laser irradiation is a serious concern in cleanrooms, where contamination of adjacent components, ejection of metal particulates, creation of void defects in the fusion zone, and significant loss of high vapor pressure alloying elements are all negative consequences of metal vaporization. Despite the widespread use of laser welding, little fundamental understanding of laser/material interaction in the weld pool exists. Without this fundamental understanding, optimization models cannot be applied to mitigate vaporization probleMs.

Important experiments on 304 stainless steel have been completed which have advanced our fundamental understanding of the magnitude and the parameter dependence of metal vaporization in laser spot welding. Experimental techniques have been developed to easily measure the laser spotsize on the sample surface, and to quantify the dependence of metal vaporization on laser beam intensity. The experiment was successful in preventing large particle ejection and actually quantified the laser beam intensities required for the onset of spatter as well as melting. Mass loss measurements were significant with up to 70 mg loss from each laser pulse. The vaporized metal has not yet been identified but additional experiments and analysis are planned to characterize the vapor, temperature fields on the weld pool surface, and develop an analytical model of the vaporization mechanism.

Keywords: Laser Welding, Laser/Material Interaction, Fusion Zone, Melting, Spatter

259. **SCIENCE BASED PROCESSING OF FIELD-STRUCTURED COMPOSITES**
$96,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Rodney L. Williamson (505) 845-3105

Field structured composites (FSCs) are anisotropic particle composites produced in a magnetic or electric field. They exhibit highly anisotropic properties due to the chain or sheet-like structures that form as a result of induced dipolar forces. By producing FSCs in a triaxial magnetic field and adjusting the relative strengths of the triaxial field components, a variety of structures can be made that cannot be produced in any other way. These include foams, chains, sheets, interpenetrating sheets, and sheets connected by chains. Such structures can be preserved by producing them in a liquid monomer which can then be polymerized in the presence of the triaxial field, or by swelling a polymer matrix with a solvent containing magnetic particles and letting the carrier solvent evaporate in the presence of the field. Field-structuring potentially enables one to produce materials with tailored material properties to meet specific needs. Recent research at Sandia has shown that these materials, when produced with electrically conductive particles, exhibit colossal changes in resistance when slightly strained or when exposed to small changes in temperature, chemical or magnetic environment. Thus, FSCs show great promise as ultrasensitive sensors if they can be reliably produced with the desired resistivity. These sensors could be made in a wide range of shapes and sizes for many different applications. The goal of this work is to learn how to actively control the structure of these materials by manipulating the field so that composites with known resistivity can be reliably and reproducibly made. Because several different structures may give rise to the same resistance, it is important to control structure so that the proper response to changing environmental factors can be achieved. This poses novel and nontrivial feedback control challenges, due to strong history effects, diverging timescales, and nonlinear dynamics.

Keywords: Field Structuring, Composites, Thermoresistance, Piezoresistance, Magnetoresistance, Chemiresistance

260. **DESIGN, SYNTHESIS, AND CHARACTERIZATION OF SOFT MATTER NANOLAYER SUPERLATTICES**
$296,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Alfredo M. Morales (925) 294-3540

Recently, birefringent polymer nanolayer superlattices that displayed enhanced reflectivities were reported in the literature. These superlattices consisted of alternating nanolayers of isotropic polymethyl methacrylate (PMMA) and either birefringent polyester or birefringent syndiotactic polystyrene. The reflectivities of the p- and spolarized light from the superlattices were determined by the indices of refraction of the nanolayers. However, as reported these superlattices are passive materials: once fabricated, the optical properties cannot be changed in response to the reflected light or to a trigger signal. This project seeks to modify by organic chemistry the composition of one of the nanolayers to include photochromic molecules that could change the indices of refraction of that set of nanolayers when triggered by an external signal. This change in refractive indices will change the overall reflectivity and the value of the Brewster angle enabling optical switching. We have synthesizing photoswitchable polymers by appending azobenzene dies to the PMMA nanolayers. The azobenzene functionality undergoes a trans-cis photoisomerization that changes the refractive index of the material. To help guide the synthetic effort, computations of optimum geometries and optical properties at the semi-empirical level are currently underway for an initial set of diazo compounds. The results will be calibrated against available experimental data to determine if the semi-empirical methods can reproduce trends in optical properties of substituted diazo compounds. Superlattice fabrication will be carried out with a modified coextruder. Ultimately, these novel materials will be used for fabricating optical microdevices such as stationary (i.e., no mechanical moving parts) optical switches.

Keywords: Superlattices, Birefringent, Nanolayers, Photochromic, Microdevices

261. **PHOTO-CONTROL OF NANO-INTERACTIONS IN MICROSYSTEMS**
$271,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Nelson S. Bell (505) 844-6234

The manipulation of physical interactions between structural moieties on the molecular scale is a fundamental hurdle in the realization and operation of nanostructured materials and high surface area microsystem architectures. These include such nano-interaction-based phenomena as self-assembly, fluid flow, and interfacial tribology. The proposed research utilizes photosensitive molecular structures to tune such interactions reversibly. This new material strategy provides optical actuation of nano-interactions impacting behavior on both the nano- and macroscales and potential impacting directed nanostructure formation, microfluidic rheology, and tribological control.

Activites will focus on the identification and examination of organic structures possessing known photophysical effects that have a high probability for influencing target interaction processes, e.g. physical entanglement, hydrophobicity/philicity, local electrostatic charge or pH changes. Their incorporation into polymeric chemistries will allow their application to inorganic colloids as photo-active surfactants. This will allow the photo-actuated control of interparticle nano-interactions in self-assembled photonic band gap structures (artificial opals). Primary demonstration of successful nano-interaction control will be provided by photo-induced modulation of the photonic band gap in the material. In addition to providing a demonstration of this fundamentally new approach for the real-time control of interfacial processes, the photo-actuation of photonic lattice material represents a new operating strategy for such photonic structures, forming the basis for beam redirection and switching devices useful in information processing systeMs.

Extension of these fundamental findings can also provide optically tuned microfluidic rheology and tribological control useful in a range of microsystems with an impact on DOE/DP technologies for stockpile safety and security.

Keywords: Photosensitive, Photonic, Rheology, Polymeric

262. **ELECTROCHEMICALLY DEPOSITED ALLOYS WITH TAILORED NANOSTRUCTURES FOR LIGA MICROMACHINES**
$336,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Dean C. Dibble (925) 294-3417

The performance of LIGA micromachines is directly linked to the mechanical, magnetic, and tribological properties of the electrodeposited alloys used in component fabrication. Surface-active compounds are used in the electrodeposition process to control grain nanostructure, composition, and internal stress of the alloy. Additives dramatically alter these properties, and can greatly enhance the mechanical strength of the component or they may contribute to undesirable effects such as fracture embrittlement. Additives for electrodeposition processes are empirically developed. More importantly, there is little, if any, physico-chemical understanding of the relationship between additive structure and electrochemical action. We propose to develop the science base needed for the rational development of alloy-deposition processes in LIGA using additives and other advanced electrodeposition techniques (such as pulsed current electrodeposition). To such effect we will develop nanoscale diagnostics that can be performed in-situ during electrodeposition. We will use these diagnostics to characterize in detail the electrodeposits at the nanometer scale. The efforts of such an investigation will be clearly focused on improving process conditions and they will be facilitated by a close collaborative effort between fundamental surface science and electrochemical engineering methods.

Keywords: LIGA, Electrodeposition, Tribological, Micromachines

263. **SOLUTION-BASED NANOENGINEERING OF MATERIALS**
$316,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: James A. Voigt (505) 845-9044

Solution-based synthesis is a powerful approach for creating nano-structured materials. We propose to develop the scientific principles required to design and build unique nanostructures in crystalline oxides and II/VI semiconductors using solution-based molecular self-assembly techniques. The ability to synthesize these materials in a range of different nano-architectures (from controlled morphology nanocrystals to surface templated 3-D structures) will provide new opportunities for the development of interactive interfaces for optics, electronics, and sensors. The wide range of interfacial nanostructures of ZnO (hexagonal rods, hollow hexagons, and oriented thin sheets) produced recently via nucleation and growth from aqueous solutions illustrates the potential of this approach. The key to controlled fabrication of such nanostructures lies in understanding the factors that control nucleation and growth processes. To achieve this understanding, we will conduct systematic nucleation and growth studies that combine: 1) synthesis using carefully controlled and monitored flow reactor systems, 2) characterization of surface chemistry and complexation, and 3) molecular modeling. Unique flow reactors will be used to control all of the critical system parameters such as supersaturation levels, hydrodynamics, and the concentrations of additives that promote nucleation and influence relative growth rates on specific crystal faces. Techniques such as Fourier Transform Infrared (FT-IR) spectroscopy, surface charge measurements, and the interfacial force microscope will be used to monitor the extent and orientation of additive adsorption and what affect such agents have on interfacial properties. Finally, surface energy calculations based on interatomic potentials will be used to model ligand adsorption on hydrated crystal surfaces. The calculations will be used to design crystallographically specific adsorbate ligands that will be synthesized and tested as surface-specific nucleation promoters and growth inhibitors

Keywords: Template, Nanostructures, ZnO, Supersaturation

264. **ASSEMBLY AND ACTUATION OF NANOMATERIALS USING ACTIVE BIOMOLECULES**
$485,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: George Bachand (505) 844-5164

The formation and functions of living materials and organisms are fundamentally different from those of synthetic materials and devices. Synthetic materials tend to have static structures, and are not capable of adapting to the functional needs of changing environments. In contrast, living systems utilize energy to create, heal, reconfigure, and dismantle materials in a dynamic, non-equilibrium fashion. The overall goal of the proposed research is to organize and reconfigure functional assemblies of nanoparticles using strategies that mimic those found in living systeMs. Active Assembly of Nanostructures will be studied using active biomolecules to create nanowires for programmable interconnects via the on-chip manipulation of gold nanoparticles. In this system, kinesin motor proteins and microtubules will be used to direct the transport of gold nanoparticles on lithographically defined array patterns such that the particles form nanowires and associated interconnects. Responsive Reconfiguration of Nanostructures will be investigated using active biomolecules to mediate the optical properties of quantum dot (QD) arrays through modulation of inter-particle spacing. Here, the spacing between different sized QDs will be controlled by activation of kinesin motor proteins, and the optical property of the surface defined by fluorescence resonant energy transfer between QDs as the inter-particle spacing is changed. In this work we will demonstrate the ability to create and reconfigure synthetic nanostructures using biomimetic process that direct energy consumption to single molecules, and remove diffusional and entropic limitations. The ability to utilize active biomolecules and nanomaterials in integrated systems could revolutionize the exploitation of nanostructures material in complex systems.

Keywords: Biomolecules, Nanowires, Nanoparticles, Functional Assemblies

265. **DECOMPOSITION OF CONTAMINANTS USING PHOTOCHEMICALLY ACTIVE NANOPARTICLES**
$396,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Kevin McCarty (925) 294-2067

The decomposition of hazardous biological (viruses and bacteria) and non-biological (e.g., nerve agents, H2S, HCN) compounds can be realized using a new class of photochemically active nanoparticles that have been fine-tuned for decontamination applications. Several metal oxides (TiO_2, ZnO, Fe_2O_3, WO_3) have demonstrated the ability to destroy contaminants upon exposure to UV light; however, to make them of practical use improvements in their activity is necessary. These materials work by photo-activating water and oxygen to create highly reactive species (e.g., OH´) that readily decompose the compounds described above. Our approach will be to develop highly photo-active, doped-nanomaterials using novel synthetic routes. We will link materials-synthesis studies to understanding the underlying physical mechanisms of these reactions through the use of in-situ microscopy and spectroscopy. These efforts will be coupled to first-principles calculations of the reaction processes and statistical mechanical modeling of the reaction dynamics. In this manner, the complex inter-relationship between nano-structure, composition, and photochemical activity will be unraveled. Directed by this understanding, sol-gel and surfactant-based supramolecular self-assembly techniques will be used to engineer optimized nanostructures with specified compositions. The photochemical activity of these improved materials will be verified by testing. The ultimate outcome of this work will be the development of new class of highly active materials for wide ranging decontamination applications.

Keywords: Nanoparticles, Photo-Active, Materials Synthesis, Decontamination

266. **THERMALLY CLEAVABLE SURFACTANTS**
$296,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Blake Simmons (925) 294-2288

Surfactants are molecules that have the ability to self-assemble into a variety of supramolecular structures. These structures, and the intrinsic amphiphilic nature of the oil-water interface they possess, have been used in numerous laboratory and industrial processes, including the synthesis of advanced materials. A major problem associated with the use of surfactants is their subsequent removal after use and the recovery of segregated materials. We propose a non-invasive approach to surfactant removal using thermally degradable surfactants that contain thermal weak-links either internal to the molecule itself or, alternatively, as a cleavable linkage between two surfactant molecules. The thermal degradation is based upon a reversible Diels-Alder reaction, which has already found utility at SNL in the preparation of removable encapsulants, foams, adhesives, and dendrimers.

Surfactant removal becomes very significant in the realm of extended mesoporous nanosized structures, such as ceramics, polymers, inorganic nanocrystals, and polymer-ceramic composites. The present technique of material recovery is typically a combination of centrifugation, calcination, and solvent washing that destroys the desired architecture and functionality of the synthesized material. The incorporation of a thermally cleavable linkage would solve this problem by allowing for the removal of the surfactant molecules through a non-invasive thermal trigger.

Initial efforts would focus on the synthesis of a surfactant that incorporates the thermal weak-link between the hydrophilic head and hydrophobic tail sections of the molecule. These two sections would then dissolve in the appropriate phase and be permanently removed from the system through thermal treatment. Phase behavior and supramolecular self-assembly of the synthesized surfactants will be computationally modeled and correlated with experimental results to develop a fundamental knowledge of these molecules. Once a working knowledge of these systems is obtained, previously unobtainable extended ceramic, polymeric and composite materials will be synthesized within these systems, recovered after thermal cleavage, and fully characterized.

Keywords: Surfactants, Mesoporous, Materials Synthesis, Diels-Alder

267. **TRANSITION-METAL CATALYZATION OF COMPLEX-HYDRIDE ABSORPTION/DESORPTION REACTIONS**
$197,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Eric Majzoub (925) 294-2498

Complex metal-hydrides, such as $NaAlH_4$, are attractive materials for hydrogen storage due to their large hydrogen capacity (5.5 wt.% for $NaAlH_4$) with respect to traditional interstitial hydrides (typically <1.5 wt.%).

These materials are currently at the forefront of a paradigm shift in energy utilization and transport. In comparison, comparable volumetric densities of compressed hydrogen gas require pressures near 10,000 psi, raising safety concerns. In addition, the current DOE goal is 7.5 wt.% H2, including container and hydride weight, excluding traditional metal-hydrides. There are two reasons for further studies of $NaAlH_4$. First, absorption and desorption kinetics in this system are enhanced by the addition of a catalyst-precursor, typically a transition-metal halide, whose fundamental mechanism is not understood. Secondly, many similar complex hydride systems, containing a larger weight percentage of hydrogen, are known. Therefore, using $NaAlH_4$ as a model system, the goal of the proposed research is to catalyze the absorption and desorption reactions and tailor the plateau pressures of a new class of metal hydrides, consisting of covalently bonded materials such as, but not limited to, $NaAlH_4$, $LiAlH_4$, $LiBH_4$, and $NaBH_4$.

The use of covalently bonded hydrogen storage systems is novel and requires a new approach to the problems of catalysis and thermodynamics. The proposed study will address two principal questions. First, can the thermodynamics of $NaAlH_4$ be tailored? This depends on the ability of the material to tolerate substitutions and vacancies in the lattice in each of the two decomposition steps encountered during desorption. Second, to what extent can the reaction be catalyzed? If a detailed knowledge of the current catalyzation process can be gained, better catalysts are likely to be found.

Keywords: Catalysis, Thermodynamics, Metal-Hydrides, Hydrogen Storage

268. **ASSEMBLY OF ORDERED ELECTRO-OPTICAL AND BIOACTIVE MATERIALS AND COMPOSITES**
$396,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Jun Liu (505) 845-9135

The discovery of intrinsic metal-like conductivity in conjugated polymers represents a significant milestone in polymer chemistry and materials science as recently recognized by the 2000 Nobel Prize Award in Chemistry. This project aims to address several key issues related to the performance and utility of conductive polymers. Our objectives are:

- To develop new methods to assemble ordered conducting materials on multiple length scales. Both self-assembly and directed nucleation and growth approaches will be explored to produce oriented and aligned polymer nanostructures and microstructures.

- To establish fundamental structure-property relationships of nanostructured conjugated polymers. We propose to investigate films in which conjugated polymers and polymer-nanocrystal composites are confined to ordered structures with 1-, 2-, or 3-dimensional connectivity and separated by either insulating or semiconducting walls. Such composites are ideal model systems in which to test and understand the role of nanostructuring in determining charge and energy transport properties.

- To integrate the new materials/structures with microelectronic/microfluidic devices. This strategy holds the promise for inexpensive electronic/optical devices. Micro-arrays of such materials will also be developed for quantitative and high sensitivity detection of chemical and biological agents. The proposed research will not only contribute to our new strategy thrust in complex functional materials, it will also have a positive impact on DOE's missions in energy and national security.

Keywords: Bioactive Materials, Electro-Optics, Microelectronics, Microfluidics, Functional Materials

269. **ACTIVE PHOTONIC NANOSTRUCTURES**
$500,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Michael Sinclair (505) 844-5506

Photonic crystals (PCs) constitute a new class of nano-engineered dielectrics that provide a novel and exceedingly powerful means for controlling photons. These artificial microstructures consist of a periodic repetition of dielectric elements which create forbidden energy bands for photons. PCs represent a major new frontier in optoelectronics due to their ability to coherently manipulate light. This manipulation is essential for new concepts such as negative indices of refraction, tailored photonic density of states, controlled spontaneous emission rates, and modified black-body radiation. PCs also promise novel applications in optical communications, computing, displays, medical diagnostics, and chemical and biological sensing.

To date, however, research in PCs has been almost entirely on "passive" structures, in which light is guided without external "active" controls. In this project, we propose to combine conventional PC nanostructures with "active" materials and/or elements that exhibit nonlinear-optical, electro-optical, piezo-electrical or electro-mechanical properties. In addition to the passive manipulation of light, such structures can provide "active" functions such as optical amplification, lasing, light switching and steering, optical logic, chemical sensing, etc.

To activate the nonlinear-optical functions of PC structures, we will incorporate semiconductor colloidal quantum dots (QDs) into 2D and 3D photonic lattices. These novel, "active" PC systems will be used to investigate the interplay between the restricted and independently tunable electronic (QDs) and photonic (PCs) densities of states. Such research could potentially lead to new types of microlasers with extremely low pump thresholds and ultra-fast modulation rates. By introducing electro-optical species into PCs, we will develop optical switches that are controlled by electrical signals. The proposed project draws upon our demonstrated strengths in PC structures, colloidal QDs, energy transfer in composites, nanomechanics, and self-assembly. This proposal invests in an important S&T area that is likely to have a strong future impact on national security missions.

Keywords: Photonics, Optoelectronics, Photonic Crystals, Active Control, Electro-Optics

270. **STUDY OF POLYMER SPIN-COATING FOR PHOTOLLITHOGRAPHIC SEMICONDUCTORS IN NEAR ZERO GRAVITY ENVIRONMENT**
$26,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Steven Thornberg (505) 844-8710

In collaboration with the University of New Mexico (UNM) and the National Aeronautics and Space Administration (NASA), we propose to investigate the feasibility of conducting the spin-coating process in a near-zero gravity environment. Using an instrument highly modified to operate under these conditions, a series of silicon wafers will undergo spin-coating with a commercial photoresist. This experimentation will be carried out aboard NASA's KC-135 aircraft housing the reduced gravity laboratory.

This unique opportunity to test the spin-coating process in a microgravity environment will provide experimental results that build on knowledge gained from the two previous years' experiments. Those experiments showed that the spin-coating process changes significantly in the absence of gravity, not only in the delivery of the photoresist to the wafer but also the distribution of the fluid across the wafer's surface. It is possible that this research will provide the data necessary for this or other processes to be adapted to space environments.

Keywords: Spin Coating, Photoresist, Micro-Gravity, Semiconductors

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

271. **MATERIALS PERFORMANCE**
$900,000
DOE Contact: Kimberly Budil (202) 586-7831
SNL Contact: William F. Hammetter (505) 272-7603

This project addresses the need to understand composition-structure-performance relationships for critical non-nuclear materials in current and proposed weapon applications. The work is focused on providing the scientific basis for materials development and optimization of properties. Due to the importance of ferroelectric materials in stockpile applications, one effort is aimed at understanding the effects of extrinsic variables such as porosity, PbO stoichiometry, and dopant type and concentration on the properties and ferroelectric-antiferroelectric phase transitions of $Pb(Zr,Ti)O_3$ ferroelectrics. In addition, as applications approach the nanoscale, it is critical to understand the effects of domain size and mobility on ferroelectric response. Complimentary work is focused on developing a quantitative model of sintering to predict densification, material compatibility and microstructure development during fabrication of complex ceramic materials, such as multilayer electronic substrates.

Keywords: Ferroelectric, Ceramic, Sintering, Nanoscale

272. **HIGH PRESSURE AND SHOCK PHYSICS**
$250,000
DOE Contact: Kimberly Budil (202) 586-7831
SNL Contact: George A. Samara (505) 844-6653

The goal of this project is to develop continuum and atomic level understanding of shock-induced phenomena in materials used in shock-activated weapons components. Together with complementary high-pressure material physics studies, this work provides new understanding of ferroelectrics and polymeric encapsulants as well as essential insights to guide performance and reliability assessments. Looking to the future, we expect that micro- and nanoscale materials will find numerous applications in nuclear weapon systeMs. Consequently, it will be necessary to measure and understand the mechanical properties, especially the shock responses, of the new materials. As a first step towards this goal, we have recently developed a new capability at Sandia, the "photonic driver", which addresses both the high per-experiment costs of current shock methods and the inability of these methods to characterize materials having very small dimensions

Keywords: Ferroelectric, Encapsulants, Nanoscale, Photonic, Shock Response

273. **AGING OF ORGANIC MATERIALS**
$1,100,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Roger L. Clough (505) 844-3492

Work on organic materials aging focuses on providing an understanding of degradation mechanisms, developing specialized analytical techniques for monitoring material aging at low levels and on short length scales, and providing methodologies for predicting material properties, reliability and lifetimes. One current thrust comprises identification and modeling of the parameters underlying radiation-induced conductivity in materials. New approaches employing isotopic labeling using C-13, O-17 and O-18, in combination with the nuclear magnetic resonance technique (NMR) or nuclear activation methods, is yielding information on chemical reactions underlying macromolecular degradation mechanisms, at an unprecedented level of detail. Work on interfaces is providing critical insights into the mechanisms of adhesion, dewetting and delamination relevant to weapon components. A variety of techniques are being employed for interfacial studies; one new technique that is particularly promising in this application is near edge X-ray absorption fine structure (NEXAFS), which is being developed to allow identification of polymer surface structure.

Keywords: Degradation, NMR, Radiation, NEXAFS, Reliability

274. **CORROSION SCIENCE AND METAL DEGRADATION**
$1,043,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contacts: Jeffrey W. Braithwaite (505) 844-7749 and Charles H. Cadden (925) 294-3650

The physical and electrical properties of metals can significantly degrade over time because of interactions with the environment. The objective of this project is to develop the mechanistic understanding and, as required, associated characterization techniques of selected corrosion-related degradation phenomena of both immediate and longer-term relevance to stockpile issues. Importantly, the advancements made in this task constitute the needed physical basis for 1) emerging analytical toolsets that will be used to predict the effects of metal aging on component service life, and 2) defining strategies that will enable real-time state-of-health sensor technologies to be developed. The processes currently being studied include: (a) corrosion of small-feature aluminum metallization features under atmospheric conditions (microelectronic devices) (b) the environmental degradation of coated and/or passivated polycrystalline silicon (surface micro-machined devices), and (c) the aging of LIGA-based microsystem materials.

Keywords: Corrosion, Passivated, Microsystem, Aging, Degradation

275. **RELIABILITY IN MICROSYSTEM MATERIALS**
$1,530,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contacts: Kevin F. McCarty (925) 294-2067
Jonathan S. Custer (505) 845-8594

This project focuses on improving the fundamental understanding of the Microstructural mechanisms that control mechanical and tribological performance over time of materials and coatings useful for both Microsystems and conventional hardware. Test methods for measuring and modeling properties of materials like fracture strength and hardness on small length scales are being developed. These methods are applied to different materials to study fracture of ceramics and braze interface reliability. The tribology, environmental reliability, and dormancy issues of surface coatings are also being explored. In addition, the changes in interface performance in microsystems are being investigated as a function of age. The central role of microstructure on the performance of stockpile components and replacement designs based on microsystems will be quantified. This project will provide tools to measure and understand materials performance at small length scales, data on mechanical properties and reliability of microsystem materials, understanding of tribological coating performance and reliability, grain boundary structure and dynamics, and materials modeling computational technique development. Results will provide quantitative input for design guides, materials model development, and for validation of model/simulation results.

Keywords: Time-Dependent, Microstructure, Electrodeposition, Lifetime, Grain-Boundary, Tribology, Microsystem, Aging

276. **NANOMECHANICS**
$250,000
DOE Contact: Larry Newkirk (202) 586-7831
SNL Contact: J. Charles Barbour (505) 844-5517

The goal of this effort is to develop a precise understanding of the high strain-rate behavior of materials at small length scales. For materials modeling, code development and implementation is done to understand the mechanical properties of materials. This modeling will ultimately link electronic and atomic-level properties to the continuum level. For materials experimentation, new methodologies of producing atomically-tailored materials and testing the mechanical response of these materials are required. In addition, new test structures are being developed with submicron-scale component features.

Keywords: Mechanical, Modeling, Atomic-Level, Mechanical, High Strain Rate

277. **MAGNETIC-FIELD EFFECTS ON VACUUM-ARC PLASMAS**
$221,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Paul A. Miller (505) 844-8879

The two main goals of this project are to understand the role of the self-magnetic field on the vacuum-arc ion source in neutron tubes and to realize magnetic shaping of the plasma plume from the ion source, thereby enabling increased plasma utilization efficiency, reduced stress on the electrode films, and reduced electrical drive requirements. Prior to this project, computational and experimental studies of neutron tubes had neglected magnetic field effects. At this point in the project, we have shown experimentally that uniform applied fields (< 300 Gauss) strongly influence the arc impedance, the shape of the plasma plume, and the total ion output. This field level is comparable to the self-magnetic field of the arc. We have studied magnetic effects computationally with the Large Scale Plasma (LSP) code. Two-dimensional magnetostatic calculations agree with some of the measurements and three-dimensional electromagnetic calculations are under development. Compact neutron tubes employ annular ion beams in order to minimize adverse defocusing effects due to the space charge of the ions in the beam. Present tubes form annular beams by geometrically selecting an annulus of the total output from vacuum-arc-plasma ion sources and discarding the rest of the plasma. If we can use magnetic fields to form plasma into an annular shape, then we can use all the plasma. More efficient use of the plasma would reduce the performance requirements on the thin-film electrodes of the vacuum arc, which provide the plasma ions, and reduce the electrical drive requirements for the ion source. Our present LSP calculations predict that a uniform axial magnetic field will produce plasma that is hollow for a short distance in front of the arc. We are presently conducting measurements to test that prediction and we will be studying tapered magnetic fields computationally to improve the annularity of the plasma.

Keywords: Vacuum-Arc Plasmas, Magnetic Fields, Plasma Plume, Langmuir Probe

278. **FIRST-PRINCIPLES DETERMINATION OF DISLOCATION PROPERTIES**
$166,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: John C. Hamilton (925) 294-2457

Dislocation behavior determines numerous materials properties. Their motion produces deformation. The interaction of dislocations with interfaces produces the grain-size dependence of strength. Motion of dislocations in boundaries determines the boundary mobility and thereby microstructural evolution. Prediction of dislocation core structures at the atomistic level in arbitrary materials and ultimately in the presences of defects is central to developing predictive models of material evolution. It would also represent a major scientific achievement.

The need to treat arbitrary materials, alloys and dopants requires a predictive first-principles approach. Current first-principles modeling capabilities are not well-suited to the description of materials properties. Techniques for determining the electronic structure of large numbers of atoms (order-N methods) work well for insulating materials but not for metallic systeMs. Further, essentially all ab-initio modeling to date employs band structure techniques with periodic boundary conditions. Thus dislocations and other aperiodic defects are difficult to model. Here we propose to adapt a combined electronic/lattice Green's technique to the direct calculation of dislocation core structures, which avoids the requirement of periodic boundary conditions. Both Green's functions exploit the short-range character of the Hamiltonians defining them. Thus, far from the core, the corresponding Hamiltonians of the host are well approximated by a slightly perturbed crystal Hamiltonian. The Green's function for the defect is solved using the Dyson equation. Additional modeling using an ab initio extension of Peierl's-Nabarro will also be pursued. The result of these calculations can be validated by detailed comparison with high-resolution electron microscopy observations. The success of this project will create a new world-class tool for the fundamental study of dislocation properties.

Keywords: Dislocations, First-Principles Modeling, Hamiltonians

279. **DYNAMICS OF METAL/CERAMIC INTERFACES**
$156,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Kevin F. McCarty (925) 294-2067

The goal of this project is to understand how metal/ceramic interfaces form, evolve, and accommodate the stress that can lead to delamination and failure. We emphasize the use of advanced microscopies such as scanning-tunneling microcopy and low-energy-electron microscopy to observe interface formation in real time. These techniques are used to measure the interfacial work of adhesion, determine the mechanisms and kinetics of interface formation, and develop understanding of how stress is or is not accommodated.

Keywords: Metal/Ceramic Interfaces, Microscopy, Adhesion

280. **IN-SITU CHARACTERIZATION OF SOFT SOLUTION PROCESSES FOR NANOSCALE GROWTH**
$96,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Nelson S. Bell (505) 844-6234

The study of novel materials and structures with dimensions in the nanoscale (<100 nm) regime is an important, emerging field of materials science. The small size of these materials results in quantum confinement and surface contributions that translate into novel opto-electronic properties whose applications are still being realized. Many synthesis techniques for nanomaterials are based on soft solution processes (SSP), which include sol-gel, hydrothermal, solvothermal, micellular or organic templating routes, and electrochemical methods. These processes involve the precipitation of ionic species or metal-organic molecules into nanoparticles or nanostructured networks. In order to exercise a high degree of control over these processes, it is critical to have a capability for monitoring the development of supersaturation, surface reactions, and formation of phase or precipitate in situ. This proposal studies the superposition of different measurement techniques to characterize dynamic colloidal systems in new ways. These studies will probe the chemical interactions during reactions, and the organizational characteristics developed in the resulting colloids. Of particular interest are properties influencing colloidal dynamics such as zeta potential and particle size development.

Keywords: Nanomaterials, Soft Solution Processes, Colloids

281. **DETERMINATION OF CRITICAL LENGTH SCALES FOR CORROSION PROCESSES USING MICROELECTROANALYTICAL TECHNIQUES**
$156,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Kevin R. Zavadil (505) 845-8442

A key factor in our ability to produce and predict the stability of metal-based macro- to nano-scale structures and devices is a fundamental understanding of the localized nature of corrosion. Corrosion processes where physical dimensions become critical in the degradation process include localized corrosion initiation in passivated metals, micro-galvanic interactions in metal alloys, and chemistry in adsorbed water films in atmospheric corrosion. This proposal focuses on two areas of corrosion science where a fundamental understanding of processes occurring at critical dimensions are not currently available.

We will study the critical length scales necessary for passive film breakdown in the inundated Al system and the chemical reactions and transport in ultra-thin water films relevant to the atmospheric corrosion of Al. Techniques are required that provide spatial information without significantly perturbing or masking the underlying relationships. Al passive film breakdown is governed by the relationship between area of the film sampled and its defect structure. We will combine low current measurements with microelectrodes to study the size scale required to observe a single initiation event and record electrochemical breakdown events. The resulting quantitative measure of stability will be correlated with metal grain size, secondary phase size and distribution to understand which metal properties control stability at the macro- and nano-scale. Mechanisms of atmospheric corrosion on Al are dependent on the physical dimensions and continuity of adsorbed water layers as well as the chemical reactions that take place in this layer. We will combine microelectrode arrays with electrochemical sensing and electrostatic force microscopy to monitor the chemistry and ion transport in these thin layers. These measurements will be the basis for calculating oxidant partition coefficients and ion mobilities. The techniques developed and information derived from this work will be used to understand and predict degradation processes in electrical and structural components.

Keywords: Corrosion Science, Microelectrodes, Degradation Processes

282. **EXPLORATION OF NEW MULTIVARIATE SPECTRAL CALIBRATION ALGORITHMS**
$148,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: David M. Haaland (505) 844-5292

We have developed a number of powerful new multivariate calibration algorithms that have been demonstrated to correct many of the outstanding limitations of traditional quantitative multivariate spectral calibrations and to greatly extend our ability to solve new probleMs. We have developed a family of augmented classical least squares (ACLS) multivariate algorithms, and we have greatly improved multivariate curve resolution (MCR) methods. The ACLS algorithms have the ability to be rapidly updated during prediction without recalibration while the MCR techniques allow us to perform multivariate calibrations without the use of standards. The rapid updating feature of the ACLS algorithms is a significant advantage over previous chemometric algorithMs. We will continue to quantify the relative merits and predictive performance of these new multivariate algorithms relative to traditional multivariate calibration methods, and we will explore exciting new potential applications using the improved MCR algorithMs. For example, the new ACLS algorithms can take advantage of weighted least squares methods to accommodate non-uniform noise in spectral data. The ability to better handle non-uniform spectral noise will be tested with simulation calibration data. The improved MCR capabilities will be used to test our hypothesis that they can be used to improve spectral calibrations that are currently limited by the reference methods required to build multivariate calibration methods. Since reference errors are often the limiting factor in multivariate spectral calibrations, reducing or eliminating this limitation would be a significant advance in chemometric data analysis capabilities. If we can successfully reduce the impact of reference errors in spectral calibrations, then we also have the opportunity to determine if the generally high precision of spectral measurements can be used to decrease errors in the primary reference methods. Success at this goal could have a very significant impact on all our instrumental analytical reference tools.

Keywords: Multivariate Calibration, Hyperspectral Image

283. **NANOSTRUCTURED MATERIALS FOR DIRECTED TRANSPORT OF EXCITATION ENERGY**
$296,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Michael B. Sinclair (505) 844-5506

One functionality that is extremely desirable for nanostructured materials is the ability to efficiently activate or interrogate structures within a nanomaterial using optical energy. However, given the packing densities obtainable with nanofabrication, direct focusing of incident optical energy onto individual nanostructures is impractical. The project will determine how the phenomenon of energy transfer can be harnessed to provide this functionality. Energy transfer is the process by which excitation energy resulting from absorption of photons can become delocalized and move from the site where the photon was absorbed. Energy transfer plays a prominent role in the photosynthetic process, where "light harvesting antennas" efficiently absorb sunlight and deliver the excitation energy to the photosynthetic reaction center. The antennas comprise arrays of absorbing organic chromophores that are coupled via near-field electromagnetic interactions. We will use the tools of nanotechnology to control the structure, and, hence, the energy transport properties of chromophore arrays. We will use nanolithography to pattern substrates in a manner that will allow us to measure the extent of delocalization in chromophore arrays. We will also use nanolithography to create site-energy and site-spacing gradients within chromophore arrays in an effort to drive excitation energy transport in predetermined directions. We will also utilize self-assembly techniques such as self-assembled monolayers and Langmuir-Blodgett films to control the growth, structure and energy transport properties of chromophore arrays. Recent theoretical investigations have lead to the prediction that surface plasmon coupling between adjacent nanoparticles in metallic nanoparticle chains can lead to energy delocalization and transport. We will fabricate metallic nanoparticle chains using both nanolithography and self-assembly. Using a variety of optical microscopies, we will develop methods to couple electromagnetic energy into these structures, and characterize their energy transport properties.

Keywords: Nanomaterial, Chromophore, Delocalization, Nanolithography

284. **THE EFFECTS OF VARYING HUMIDITY ON COPPER SULFIDE FILM FORMATION**
$196,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: John P. Sullivan (505) 845-9496

Atmospheric corrosion of electrical components has been linked to a significant number of materials-related issues for the nuclear weapons stockpile. Further, the increasing use of Cu in commercial systems will require a long-term commitment to understand Cu corrosion mechanisms in order to reliably predict corrosion rates for commercial off-the-shelf (COTS) discrete components in the future stockpile. This project will study the effects of varying relative humidity (RH) in the sulfidation of copper - a demonstrated and recurring corrosion problem for electrical devices. The complex interactions between a sulfidizing environment and an oxidized Cu surface are dependent upon RH and temperature. Small changes in the ambient temperature near room temperature may cause significant changes in the sulfidation mechanism that can lead to greatly differing morphology of the corrosion product layer. This corrosion product layer, primarily Cu_2S, can impede mechanical functions of connectors and switches and alter the performance of electrical components. A detailed study of the critical steps during the initial stages of water layer adsorption on an oxidized copper surface and subsequent Cu sulfidation will allow identification of the relevant mechanisms governing the sulfide nucleation and growth processes. Our measurements will identify critical kinetic processes in the initial stages of growth, in order to ultimately obtain quantitative, predictive models of Cu sulfidation. This project is the most effective method to focus research efforts onto a study of the effects of varying humidity on copper sulfide film formation, and to provide the freedom to pursue the high-risk/high-payoff experiments proposed herein.

Keywords: COTS, Sulfidation, Corrosion, Humidity

285. **QUANTIFICATION OF ENVIRONMENTS AND SURFACES WITHIN MICRO-PACKAGES**
$371,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Steven Thornberg (505) 844-8710

Chemical and physical materials-aging processes can significantly degrade the long-term performance and reliability of dormant microsysteMs. This degradation results from materials interactions with the evolving microenvironment by changing both bulk and interfacial properties (e.g., mechanical and fatigue strength, interfacial friction and stiction, electrical resistance). Eventually, device function is clearly threatened and, as such, these aging processes are considered to have the potential for high (negative) consequences.

Currently, there is no reliable information on the critical species (and concentration levels) that will be present within the sealed packages or on the component surfaces. The analytical techniques for properly characterizing these environments do not exist. The goal of this proposal is to develop a set of tools that are analytical strategies and methods to measure the spatially resolved chemical inventory within a Sandia fabricated and packaged microsystem. These tools can be broadly subdivided into surface and internal gas atmosphere characterization, with the aid of multivariate data processing. Both will require the design and fabrication of a suitable microelectromechanical system (MEMS) test platform capable of being opened easily and cleanly. Surface characterization will involve labeling (e.g., isotopic, chemical tagging) known contaminants in order to monitor their movement using enhanced surface analyses. For internal gas characterization, we will develop new micro-volume sampling techniques that provide greatly enhanced sampling efficiency of analytes and couple these to mass spectrometric and optical analysis methods. We will develop and apply new multivariate statistical techniques to spatially resolved ion, x-ray and optical spectroscopies to identify and quantify the spatial distribution of critical surface species (e.g., lubricants, anti-stiction reagents) and contaminants. Tools developed in this work will enable the acquistion and processing of surface/gas data to support design of integrated state-of-health sensors, identify important degradation/dormancy mechanisms, establish packaging specifications to assure adequate weapons reliability, and establish future surveillance methods.

Keywords: Materials Aging, MEMS, Microelectromechanical, Packaging, Surface Analysis, Chemical Analysis

286. **FUNDAMENTAL MECHANISMS OF MECHANICAL RESPONSE FOR NANOSTRUCTURED MATERIALS**
$100,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Sean Hearne (505) 845-0804

Predictable performance and reliability of Sandia technologies need to be based upon fundamental mechanistic understanding and modeling. This is especially critical for introducing nanostructured materials into future generations of integrated micro- and nano-systems within the DOE complex. Therefore, a fundamental understanding of the mechanical response of nanostructured materials under these conditions is required to predict their performance and reliability. To address this, we will investigate the fundamental deformation properties of ultra-fine grain film materials such as Al, Ni, and Cu, which are important in critical LIGA and RF MEMS applications. Our objective is to determine the limits of classical scaling laws and formulate a new understanding of the mechanical response as the grain sizes are refined to nanometer scale. Previous efforts to investigate the mechanical properties of nanostructured materials were impeded by difficult, highly specialized loading conditions and a limited ability to directly image defect evolution under well-established loading conditions. In this investigation, we propose to develop and utilize a new technique for in-situ characterization to understand the critical role of defects such as dislocations, grain boundaries, and voids, in the deformation response and fracture of nanocrystalline materials. Specifically, a novel surface micromachined tensile tester fitted within a transmission electron microscope will permit direct quantitative measurements of the microstructural deformation evolution under well-characterized mechanical and thermal loading conditions. Molecular dynamic simulations will be used to examine the role of surfaces and interfaces in ultra-fine-grains materials. These results will be used to develop quantitative and predictive models of the defect interactions that govern the mechanical response within nanostructured materials. It will also establish the testing protocols required to study alloy strengthening of metals critical to the needs of LIGA. This LDRD will result in a science-based infrastructure to enhance Sandia's leadership role in research, development and mechanical reliability of nanostructured materials.

Keywords: Nanostructured Materials, Nanocrystalline, Materials Mechanics, Microstructure

MATERIALS STRUCTURE AND COMPOSITION

287. **THE BASICS OF AQUEOUS NANOFLUIDICS: "INTERPHASE" STRUCTURE AND SURFACE FORCES**
$296,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Peter J. Feibelman (505) 844-6706

To understand flow through narrow pores, biomaterials properties, micro-machine operation and other key nanofluidic phenomena, we need to learn how the unexpectedly strong forces measured as far as tens of nanometers from water-solid interfaces are mediated by near-surface water structure. Using ab-initio calculations and a suite of incisive experiments, we will identify and characterize ice-like, clathrate-like and possibly other arrangements of water molecules in the "interphase" adjacent to ice-nucleating, hydrophobic and intermediate surfaces. The measurement techniques, including infrared spectroscopy, interfacial force microscopy, contact angle studies, will illuminate the relations among interphase structure and energetics, mechanical properties and hydration forces. Our theoretical efforts will target an explanation of how templates produced by strong short-range interactions nucleate near-surface ordering of water molecules. For this purpose, we will develop and deploy a computational scheme in which the near-surface transition region is described by a classical water potential, specifically designed to reproduce the ab-initio phases and properties of bulk water, while an ab-initio description of the immediate surface vicinity provides a boundary constraint amounting to a template. After initial work in which novel experimental and theoretical methods are developed and validated, we will apply theory and experiment concurrently to a set of representative cases, including an AgI surface (epitaxy with ice), a clean metal and a self-assembled-monolayer-covered (oily) surface. We will thus learn the microscopic underpinnings of the relation between hydration force strength, surface chemistry (e.g., hydrophilicity) and physics (e.g., epitaxial match).

Keywords: Water, Ice-Like, Clathrate-Like, Ab-Initio, Monolayer

288. **MODELING LOCAL CHEMISTRY IN THE PRESENCE OF COLLECTIVE PHENOMENA**
$166,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Normand A. Modine (505) 844-8412

Many materials science problems are characterized by the interplay of two phenomena: chemical specificity (CS), controlled by the detailed behavior of chemical bonds, and collective phenomena (CP), where new behavior emerges from many body interactions. We are developing the world's first robust and efficient model bridging the length scales involved in these phenomena. In order to maintain a preeminent focus on materials science, we apply our approach to obtain an unprecedented understanding of the interplay between chemistry and collective phenomena during the aging of a complex material system, Zeolite-3A-based desiccants. Such investigations require a coupling of quantum mechanical (QM) methods and classical methods into the same simulation since classical simulation techniques alone cannot model CS reliably, while QM methods alone are incapable of treating the extended length and time scales characteristic of CP. In typical situations, where the reactions responsible for CS are localized, while the weaker, longer range interactions involved in CP can be classically represented, an efficient QM-to-classical coupling can be obtained by exploiting the natural spatial locality of electronic structure (Kohn's nearsightedness). In addition to the aging and reliability of desiccants, our model eventually could be applied to problems such as 1) Science-based processing for ceramic/metal joints, e.g., in neutron tubes, where the relationship between chemical composition (CS) and interface integrity (CP) is poorly understood; and

2) Proteomics, where active sites (CS) interact with a complex background consisting of the rest of the protein and its aqueous environment (CP).

Keywords: Collective Phenomena, Chemical Specificity, Quantum Mechanical

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

289. **ASSURING ULTRA-CLEAN ENVIRONMENTS IN MICRO-SYSTEM PACKAGES: IRREVERSIBLE AND REVERSIBLE GETTERS**
$361,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Leroy L. Whinnery (925) 294-3410

Microsystems are currently being evaluated as possible replacements for a number of weapon subsystems with the expectation of improved surety combined with reduced weight and volume. However, there is great concern that long periods of dormant storage may impair the mechanical functioning of microdevices that are exposed to water, out gassing products (organics, solvents and silicones) and particulates (talc and dust). Low temperature operating environments and small moving parts in contact with stationary and mating structures make capillary condensation, ice formation and corrosion true concerns for microsysteMs. Past experience provides little guidance, and the desiccants currently used to manage system-wide moisture levels cannot be relied on to provide the more stringent control needed to assure microsystem reliability.

We are developing a new generation of irreversible, chemically reacting getters specifically targeted toward assuring the integrity of the local environment within microsystem packages. We intend to incorporate volatile species into a polymer through covalent bonds, thus producing a non-volatile product. These reactive getters will be combined with getters that rely on absorption media (e.g., zeolites and high surface area carbon fibers) to scavenge non-reactive species, like solvents. Our getter systems will rely on device packaging to limit exchange between the microsystem and the global weapon environment. Thus, the internal getters need only provide local environmental control within the microsystem package. If the getters themselves are not tacky, they will be incorporated into a tacky polymer matrix to immobilize micro-particles in a harmless location. Modeling and analysis of available data will be used to estimate the ingress of undesirable species as well as the gettering rates, capacities, and geometries needed to maintain an acceptable environment within the package. To summarize, we propose to develop getters that utilize chemical reactions, adsorption and physical adhesion to assure a benign dormancy environment within microdevice packages.

Keywords: Getter, Microdevices, Packaging, Absorption

290. **MECHANICS AND TRIBOLOGY OF MEMS MATERIALS**
$266,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Michael T. Dugger (505) 844-1091

Micromachines have the potential to significantly impact future weapon component designs as well as other defense, industrial, and consumer product applications. For both electroplated (LIGA) and surface micromachined (SMM) structural elements, the influence of processing on structure, and the resultant effects on material properties are not well understood. The behavior of dynamic interfaces in present as-fabricated microsystem materials is inadequate for most applications and the fundamental relationships between processing conditions and tribological behavior in these systems are not clearly defined. We intend to develop a basic understanding of deformation, fracture, and surface interactions responsible for friction and wear of microelectromechanical system (MEMS) materials. This will enable needed design flexibility for these devices, as well as strengthen our understanding of material behavior at the nanoscale. The goal of this project is to develop new capabilities for sub-microscale mechanical and tribological measurements, and to exercise these capabilities to discover fundamental knowledge of material behavior at this size scale. Novel micro-force and displacement sensors using SMM technology and new methodologies for isolating local variations in mechanical response of MEMS materials will be developed. Understanding the nanomechanics of surface contact is expected to result in new fundamental contributions to theories of interfacial adhesion as a function of topography. The ability to quantify friction over a wide range of pressure and velocity conditions, and in controlled environments, will enable fundamental understanding of the effect of environment on friction and surface durability. Increased understanding of MEMS mechanics and tribology developed in this project will permit performance and reliability of advanced MEMS components to be predicted with a sound scientific basis.

Keywords: Micromachines, Interfaces, Tribology, Surface Interactions

291. **LIGA MICROSYSTEMS AGING: EVALUATION AND MITIGATION**
$356,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Charles H. Cadden (925) 294-3650

The deployment of LIGA structures in DP applications requires a thorough understanding of potential long term physical and chemical changes that may occur during service. While these components are generally fabricated from simple metallic systems such as copper, nickel and nickel alloys, the electroplating process used to form them creates microstructural features which differ from those found in conventional (e.g., ingot metallurgy) processing of such materials. Physical changes in non-equilibrium microstructures may occur due to long term exposure to temperatures sufficient to permit atomic and vacancy mobility. Chemical changes, particularly at the surfaces of LIGA parts, may occur in the presence of gaseous chemical species (e.g., water vapor, HE off-gassing compounds) and contact with other metallic structures. We propose to characterize LIGA materials currently being produced, including pure Ni, Ni-Co and Ni-Fe alloys. This baseline characterization will be used as a reference point as we monitor changes that occur in LIGA structures over extended time periods in environments similar to those envisioned for DP applications. Finally, conformal coating systems will be investigated as needed to combat environmental degradation occurring at LIGA surfaces.

Keywords: LIGA, Electroplating, Non-Equilibrium Microstructures

292. **ADVANCED PACKAGING/JOINING TECHNOLOGY FOR MICROSYSTEMS**
$321,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Charles Robino (505) 844-6557

It is generally agreed that current microelectronics packaging technologies are inadequate for potential microsystems applications. Additionally, the capability to join Microelectro Mechanical Systems (MEMS) components into complex, 3-dimensional assemblies, will be necessary for stockpile applications. Proof-of-concept experiments have identified two complementary new technologies: 1) micron-scale high energy density (HED) fusion welding and 2) focused-ion-beam deposition joining (FIBDJ) that could jointly address these key microsystem needs. At the micron scale, materials properties which dominate joining response will differ from those at macroscopic sizes. This project will identify and quantify the materials properties/process interactions which control microscale joinability in HED welding and FIBDJ.

Microscale HED welding will be studied with concurrent experimental and modeling approaches. Laser and electron beams will be characterized spatially and temporally, and in terms of energy transfer. Previous modeling has shown that melt ejection may preclude joining at <100 micron beam diameters, but did not incorporate the effect of surface tension. Model improvements will incorporate this effect and use Molecular Dynamics simulations to provide surface tensions. Surface Evolver (SE) simulations will guide experiments, and determine if recoil pressure can be used to aid coalescence. Expected results are quantitative mechanistic descriptions of microscale fusion welding, and definitions of microscale weldability.

FIBDJ will be evaluated as an alternative approach. Experiments will include characterization of operating parameters, joint geometry, energy transfer, and development of microstructure and properties. Interpretation of microstructural evolution, and its relation to FIBDJ processing will be aided by Kinetic Monte Carlo modeling. The models will be used to derive quantitative mechanistic descriptions of micron and sub-micron size FIBDJ connections and to optimize processing.

Residual stress and distortion is expected to be a key issue. We will address its impact at the latter stages of the project.

Keywords: Advanced Packaging, Microscale Welding, MEMS, Focused Ion Beam

293. **MAGNETOSTRICTIVE ELASTOMERS FOR ACTUATORS AND SENSORS**
$146,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Dale Huber (505) 844-9194

There is a need for soft actuators that have a much larger response than piezoelectrics, and that can respond in microseconds. Applications include artificial muscles in robots and stress/strain sensors based on permittivity or permeability changes. We have shown theoretically that large magnetostrictive effects can be obtained from composites of magnetic nanoparticles in an elastomer, if the nanoparticles have been preorganized into chain-like agglomerates using magnetic fields. Such Magnetostrictive Elastomers (MEs) have a magnetic permeability that increases rapidly with compression, and so contract in a magnetic field, providing the particles are spaced by a soft matrix. This effect should be especially large for nanoparticles, where calculations show that the stresses should be comparable to that of human muscle. "Latched" MEs could also be made with particles having large magnetic remanence. A short magnetic pulse would magnetize the particles, causing permanent composite contraction without further power consumption, until an opposing coercive pulse removes the magnetization, releasing the contraction. One challenge in realizing MEs is preventing contact between magnetic nanoparticles during chaining. The most effective method of precoating the nanoparticles with a thin layer of low-modulus elastomer is through a surface-initiated polymerization, wherein an initiating group covalently linked to the surface is used to grow polymers in situ, forming a defect-free coating. MEs should have wide application as large strain actuators, and as soft sensors for robotic fingertips. We expect strains that are 10-100x that of piezoelectrics, and stress response times limited only by the inductance time of the coil.

Keywords: Magnetostrictive Elastomers, Magnetostriction, Permeability, Magnetism

INSTRUMENTATION AND FACILITIES

294. **ADVANCED ANALYTICAL TECHNOLOGY PROJECT**
$990,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contacts: Raymond P. Goehner (505) 844-9200
and James Wang (925) 294-2786

Our goal is to advance the state of the art in materials characterization relevant to Defense Programs by significantly enhancing the sensitivity of existing capabilities and developing advanced analytical tools. We are developing advanced analytical sensors and techniques to detect the early indications of aging in materials that will enable the detection and quantification of the chemical and physical mechanisms that cause materials properties to change with time. Areas of emphasis include: 1) techniques using electron, x-ray, neutron and ion beams to perform structural, chemical and phase analysis on the nanometer to micron scale of complex materials and surfaces of micro-system components; 2) application and development of spectrum imaging techniques applied to electron microscopes and surface analytical techniques; and 3) improvements in optical and mass spectrometry techniques to probe subtle chemical changes that take place as materials in weapon systems age.

Keywords: Sensors, Aging, Structural Characterization, Chemical Analysis, Electron Microscopy

295. **INFORMATION EXTRACTION**
$400,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Nancy B. Jackson (505) 845-7191

Creating and applying new algorithms for the analysis of spectroscopic and materials characterization data is the focus of this project. These algorithms are the basis of improved multivariate analysis methods that have applications in polymer aging, microsystems, process monitoring, chemical analysis techniques, quality control, sensors, and remote sensing. Software will be developed that will allow expert and non-expert alike to be able to incorporate Sandia state-of-the-art Multivariate Curve Resolution (MCR) algorithms in the analysis of images. Applications using these algorithms will be used to improve developed analytical instruments including Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS), X-ray photoelectron spectroscopy (XPS), and Auger Electron Spectroscopy (AES), and for developing new analysis tools such as photoacoustic infrared spectroscopy (PAS).

Keywords: Algorithms, Multivariate Analysis, Spectroscopy

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

296. **ENGINEERED NANOSTRUCTURE LAMINATES**
$8,500,000
DOEContact: Bharat Agrawal (301) 903-2057
LLNL Contact: Troy W. Barbee, Jr. (925) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one or two dimensions during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2nm) to hundreds of monolayers (>100nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500 mm thick samples have been synthesized for mechanical property studies of multilayer structures, energetic materials development, advanced optics development and scientific studies of compound and alloy thermodynamics.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately >50 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: IR, Vis, UV, EUV, soft X-ray and X-ray optics for spectroscopy and imaging; energetic materials, high performance capacitors for energy storage; capacitor structures for industrial applications; high strength materials; integrated circuit interconnects; projection X-ray lithography optics, light weight optic systems.

Keywords: Precision Thin Films, Multilayer/Nano-Laminate Technology, Passive Electronic Devices, Energetic Materials, IR, Visible, UV, EUV, SXR and XR Optics, Optic Systems

INSTRUMENTATION AND FACILITIES

297. **AFM INVESTIGATIONS OF BIOMINERALIZATION**
$113,000
DOE Contact: Nick Woodward (301) 903-4061
LLNL Contact: J. J. DeYoreo (925) 423-4240

Living organisms use organic modifiers of nucleation and growth to control the location, size and shape of mineralized structures. While much is known about the macroscopic impact of these growth modifiers or has been inferred about the microscopic interfacial relationships between the modifiers and crystal surfaces, the atomic-scale mechanisms of biomineralization are poorly understood. In this project we use atomic force microscopy, molecular modeling and surface spectroscopy to investigate the effects of small inorganic and organic growth modifiers as well as proteins and their sub-segments on the growth of single crystal surfaces from solution. From these measurements we seek to determine growth mechanisms, geometrical relationships, and the effect on the thermodynamic and kinetic parameters controlling growth morphology and rate.

Keywords: Biomineralization, Atomic Force Microscopy, Crystal Growth

298. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$1,300,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contacts: R. Cook (925) 422-3117 and Steve Letts (925) 422-0937

This program has as its objective the development of a vapor deposition based polyimide coating technology to produce a smooth 150 µm polyimide ablator coating on a 2mm diameter capsule target for the National Ignition Facility (NIF). The approach involves first vapor depositing monomeric species to form a polyamic acid coating on a spherical hollow mandrel. The surfaces of these coated mandrels are then smoothed by exposure to dimethyl sulfoxide vapor while being levitated on a nitrogen gas flow. The smoothed shells are then heated *in situ* to imidize the coatings. During the past year shells with surfaces that meet the design requirements for NIF targets have been produced.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

299. **BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS**
$500,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contacts: R. Cook (925) 422-3117, R. Wallace (925) 423-7864, M. McElfresh (925) 422-8686

This program has as its objective the development of materials and processes that will allow sputter-deposition of up to 200 µm of a uniform, smooth, high-Z doped Be-based ablator on a spherical hollow mandrel. Capsules made with this type of ablator have been shown by calculation to offer some important advantages as ignition targets for the National Ignition Facility (NIF). Emphasis in the past year has been on improving coating homogeneity and smoothness by reducing grain size and developing laser drilling techniques that will be needed for capsule filling.

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

300. **USING DIP-PEN NANOLITHOGRAPHY TO ORDER PROTEINS AND COLLOIDS AT SURFACES**
$420,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contact: J. J. DeYoreo (925) 423-4240

The ability to organize nanometer scale species such as quantum dots, proteins, colloids and viruses is emerging as a key area of nanoscience and technology. In this project we are using dip-pen nanolithography to pattern surfaces at the nanoscale in order to create templates for assembly of ordered arrays. We are utilizing “inks” covalently bind to the “paper” (i.e., the substrate) and that ensure chemo-selective binding of the target species to the pattern. By shrinking the pattern to sufficiently small size we will be able to assemble single molecules or colloidal species into well defined arrays. The degree of ordering in those arrays will then be investigated using synchrotron methods and the assembly process itself will be modeled using kinetic Monte Carlo simulations

Keywords: Dip-Pen Nanolithography, Atomic Force Microscopy, Templates, Nanoscale Patterns

301. **PLASMA POLYMER COATING TECHNOLOGY FOR ICF TARGETS**
$600,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contacts: R. Cook (925) 422-3117 and Steve Letts (925) 422-0937

This program has as its objective the development of a CH or CD based plasma polymer coating technology to produce both thin-walled, temperature stable mandrels as well a smooth 150 µm thick CH or CD ablator coating resulting in a 2mm diameter capsule target for the National

Ignition Facility (NIF). The approach involves first forming a symmetric 2mm diameter shell mandrel from poly(a-methylstyrene) by microencapsulation. This is then overcoated with a thin (12-15 µm) layer of CH or CD plasma polymer formed by flowing a feed gas (CH_4, C_4H_6, or deuterated analogs) plus H_2 (or D_2) through an R/F field to form molecular fragments which coat the shell in a bounce pan. Pyrolysis of the poly(amethylstyrene) to gaseous monomer that diffuses away leaves the spherically symmetric, thermally stable CH or CD shell behind. Additional coating to 150 µm gives a NIF capsule target. During the past year 2-mm diameter mandrels that routinely meet the NIF surface requirement have been prepared.

Keywords: Polymers, Laser Fusion Targets, Plasma Polymer, Ablator

OFFICE OF FOSSIL ENERGY

	FY 2003
OFFICE OF FOSSIL ENERGY - GRAND TOTAL	$12,020,000
OFFICE OF ADVANCED RESEARCH	$12,020,000
ADVANCED RESEARCH MATERIALS PROGRAM	$6,049,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,539,000
Novel Processing of Mo-Si Alloy (AMES-2)	150,000
Influence of Processing on Microstructure and Properties of Iron Aluminides and Coatings (INEL-2)	170,000
Chemically Vapor Deposited YSZ for Thermal and Environmental Barrier Coatings (ORNL-1A)	225,000
Corrosion-Resistant Ceramic Coatings (ORNL-1B)	275,000
Extended-Lifetime Metallic Coatings for High-temperature Environmental Protection (ORNL-2B)	210,000
Evaluation of Advanced Pressure Boundary Alloys for Heat Recovery Systems (ORNL-2C)	240,000
Multi-Phase High-Temperature Alloys (ORNL-2D)	110,000
Development of Novel Activated Carbon Composites (ORNL-3B)	350,000
Controlled Oxidation for Functional and Protective Surfaces (ORNL-4A)	150,000
CRADA on Thermie Alloy Processing (ORNL-5M)	70,000
Development of a Commercial Process for the Production of Silicon Carbide Fibrils (REMAXCO-5)	125,000
Alluminide Coatings for Power-Generation Applications (TTU-2)	85,000
Modeling of CVD Zirconia for Thermal Barrier and Environmental Barrier Coatings (UOL-1)	229,000
Mo-Si Alloy Development (ORNL-2I)	150,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,130,000
Development of Nondestructive Evaluation Methods for Structural and Functional Materials (ANL-1)	215,000
Corrosion and Mechanical Properties of Materials in Combustion and Mixed-Gas Environments (ANL-4)	175,000
In-Plant Corrosion Probe Tests of Advanced Austenitic Alloys (FW-5)	80,000
Effect of Chromium on Fe/Al Weld Overlay Coatings for Corrosion Protection (LU-2)	100,000
Oxide Dispersion Strengthened (ODS) Alloys (ORNL-2E)	230,000
Concepts for Smart Protective High-Temperature Coatings (ORNL-4C)	70,000
Defect Content in ODS Alloys (UL-2)	100,000
Materials Testing in Fossil Energy Systems (UNDEERC-4)	100,000
Integrated Research for Predicting Higher Dimensional Phase Diagrams with Emphisis on Ternary Diagrams of Molybdenum (WVU-2)	60,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,380,000
Metallic Filters for Hot-Gas Cleanup (AMES-3)	90,000
Low-Chrome/Chrome-Free Refractories for Slagging Gasifiers (ARC-1)	200,000
Development of Ceramic Membranes for Hydrogen Separation (ORNL-3B)	350,000
Efficient Production of Hydrogen Using Pd Membrane Reactors (LANL-3)	100,000
Materials and Components in Fossil Energy Applications Newsletter (MCNL-5)	60,000[21]

[21]Matching funding provided by EPRI.

OFFICE OF FOSSIL ENERGY (continued)

	FY 2003
OFFICE OF ADVANCED RESEARCH (continued)	
ADVANCED RESEARCH MATERIALS PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
High-Temperature Materials Testing in Coal Combustion Environments (NETL-4)	150,000
Economical Fabrication of Membrane Materials (ORNL-3H)	225,000
Management of the Advanced Research Materials Program (ORNL-5A)	400,000
Development of Seals for Membranes (PNL-3)	450,000
Personal Services Contract	20,000
Development of ODS Alloy for Heat Exchanger Tubing (SMC-2)	160,000
Optimization of ODS Alloy Properties (UCSD-2)	100,000
Study of the Fatigue and Fracture Behavior of Cr-Based Alloys and Intermetallic Materials (UT-2A)	75,000
ULTRA-SUPERCRITICAL STEAM POWER PLANT RESEARCH	$1,570,000
Ultra-Supercritical Steam Turbine Materials (ARC-2)	200,000
Materials for Ultra-Supercritical Steam Power Plants (FEAA061)	1,020,000
Ultra-Supercritical Steam Cycle Turbine Materials (FEAA069)	350,000
ADVANCED METALLURGICAL PROCESSES PROGRAM	$4,401,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$901,000
Advanced Foil Lamination Technology	600,000
Advanced Casting Technologies	301,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,500,000
Advanced Refractories for Gasifiers	900,000
Oxidation and Sulfidation Resistant Materials	600,000
Wear and Abrasion of Materials for Fossil Energy Systems	600,000
Mechanisms of Corrosion Under Ash Deposits	750,000
Non-Isothermal Corrosion and Oxidation	300,000
Corrosion Resistant New Materials for Solid Oxide Fuel Cell Interconnects	350,000

OFFICE OF FOSSIL ENERGY

The Office of Fossil Energy responsibilities include management of the Department's fossil fuels (coal, oil, and natural gas) research and development program. This research is generally directed by the Office of Coal Technology, the Office of Gas and Petroleum Technology, and the Office of Advanced Research and Special Technologies in support of the National Energy Strategy Goals for Increasing Energy Efficiency, Securing Future Energy Supplies, Respecting the Environment, and Fortifying our Foundations. Three specific fossil energy goals are currently being pursued:

1. The first is to secure liquids supply and substitution. This goal targets the enhanced production of domestic petroleum and natural gas, the development of advanced, cost-competitive alternative fuels technology, and the development of coal-based, end-use technology to substitute for oil in applications traditionally fueled by liquid and gaseous fuel forms.

2. The second is to develop power generation options with environmentally superior, high-efficiency technologies for the utility, industrial, and commercial sectors. This goal targets the development of super-clean, high-efficiency power generation technologies.

3. The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

OFFICE OF ADVANCED RESEARCH

ADVANCED RESEARCH MATERIALS PROGRAM

Fossil Energy materials-related research is conducted under the Advanced Research Materials Program. The goal of the Fossil Energy Advanced Research Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systeMs. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of the DOE-FE Vision 21 concept, which aims to address and solve environmental issues and thus remove them as a constraint to coal's continued status as a strategic resource.

The principal development efforts of the Program are directed at ceramic composites for high-temperature heat exchanger applications; new corrosion- and erosion-resistant alloys with unique mechanical properties for advanced fossil energy systems; functional materials such as metal and ceramic hot-gas filters, gas separation materials based on ceramic membranes (porous and ion transport), fuel cells, and activated carbon materials; and corrosion research to understand the behavior of materials in coal-processing environments. In cooperation with DOE-ORO, Oak Ridge National Laboratory has the responsibility of the technical management and implementation of all activities on the DOE Fossil Energy Advanced Research Materials Program. DOE-FE administration of the Program is through the National Energy Technology Laboratory and the Advanced Research Product Team.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

302. **NOVEL PROCESSING OF Mo-Si ALLOY (AMES-2)**
$150,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
J. H. Schneibel (865) 574-4644
Ames Laboratory Contact: M. J. Kramer
(515) 294-0276

The purpose of this task is to evaluate the use of Mo foil as a substrate for spray-deposited Mo-Si-B alloys. One side of the foil will be sprayed with Mo-rich Alloy 3, while the other side will be sprayed with Si-rich Alloy 1. The sandwich structure will then be annealed at elevated temperature in inert atmosphere to evaluate the microstructural/phase stability of the coatings. Annealing in air will show the oxidative stability of the individual coatings and their ability to protect the oxygen sensitive Mo foil.

Keywords: Coatings, Alloys, Molybdenum, Silicon, Foil

303. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF IRON ALUMINIDES AND COATINGS (INEL-2)**
$170,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
Idaho National Engineering and Environmental Laboratory Contact: R. N. Wright (208) 526-6127

Thermal cycling experiments have shown that minimum total residual stress gives rise to the best coating performance in thermal cycling in an oxidizing environment. This is in contact with a commonly held belief in the industry that compressive stress yields better performance. Large compressive stresses correlate with coating failure by fracture and spallation between coating layers parallel to the substrate/coating interface. Coatings with large tensile stresses also fail after relatively few thermal cycles; however, the failure in these coatings occurs by debonding of the coating from the substrate. Numerical simulation of brittle materials, as the iron aluminides tend to be in the thermal spray coatings, has indicated that large compressive stresses in the plane of the coating can in fact give rise to cracking parallel to the interface. It is not likely that such a failure mechanism would be observed for ductile compositions. It is probably significant for most classes of coatings designed for high temperature coal combustion conditions.

Stresses during thermal cycling are largely a result of differences in coefficient of thermal expansion. The low residual stress coatings also tend to have lower compliance due to some porosity. This may also affect coating performance. We intend to investigate the individual contributions of stress and porosity as part of the coating performance evaluation that includes mechanical properties of the coating and strain to failure of the coating/substrate couple.

Thermal gravimetric testing equipment has been installed and experiments have begun to examine the resistance of coatings to simulated coal combustion environments. Both aluminides and Mo-Si alloys are being examined both with respect to corrosion behavior (weight loss or gain) and microstructural evolution. Many coating failures appear to initiate at the interface as noted above. The ongoing experiments will help elucidate the relative contributions of stress and corrosion on coating failure.

Keywords: Aluminides, Processing, Microstructure

304. **CHEMICALLY VAPOR DEPOSITED YSZ FOR THERMAL AND ENVIRONMENTAL BARRIER COATINGS (ORNL-1A)**
$225,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: T. M. Besmann (865) 574-6852

The purpose of this task is to develop a chemical vapor deposition (CVD) process for fabricating yttria-stabilized zirconia (YSZ) for thermal and environmental barrier applications. YSZ has been the phase of choice for thermal barrier coating (TBC) applications due to its low thermal conductivity and high thermal stability. The CVD process being explored utilizes organometallic precursors flowing over a heated substrate in a flow reactor. A current technology for thermal barrier coatings (TBCs) for high-performance turbine blades utilizes electron-beam physically vapor deposited (EBPVD) yttria-stabilized zirconia (YSZ). The deposits are columnar in nature, resulting in excellent strain tolerance during thermal cycling. There exist, however, a number of issues with regard to cost, long-term stability, and environmental degradation of these coatings. The CVD process for YSZ is being developed for consideration as a replacement for the capital intensive EBPVD process, as a supplement to EBPVD to coat regions that the line-of-sight process cannot reach, and as a seal coat (environmental barrier coating or EBC) for EBPVD layers.

Keywords: Composites, Ceramics, Coatings

305. **CORROSION-RESISTANT CERAMIC COATINGS (ORNL-1B)**
$275,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: B. A. Armstrong (865) 241-5862

The purpose of this program is to develop ceramic coatings with enhanced corrosion resistance through improvements in the composition and processing of the coating. Processing innovations will focus on aqueous coating development including such techniques as spray coating, dip coating and vacuum infiltration. Approaches to coatings, such as mullite, that have shown good corrosion resistance and materials that form scales other than silica will be evaluated. Candidate materials will be exposed in facilities at ORNL, the DOE National Energy Technology Laboratory, and the University of North Dakota Energy and Environmental Research Center. All specimens will be characterized at ORNL to identify the most promising materials for specific applications.

Keywords: Ceramic, Coatings, Corrosion

306. **EXTENDED-LIFETIME METALLIC COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL PROTECTION (ORNL-2B)**
$210,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact:
P. F. Tortorelli (865) 574-5119

The purpose of this task is to examine important composition and microstructure issues associated with the development of extended-lifetime corrosion-resistant metallic coatings for high-temperature applications associated with the key technologies of the Office of Fossil Energy's Vision 21 concept.

Keywords: Coatings, Corrosion

307. **EVALUATION OF ADVANCED PRESSURE BOUNDARY ALLOYS FOR HEAT RECOVERY SYSTEMS (ORNL-2C)**
$240,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
R. W. Swindeman (865) 574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature components in advanced combined-cycle and coal-combustion systems with emphasis on cycles at temperatures of 700˚C and higher.

Keywords: Alloys, High-Temperature Components, Combustion Systems

308. **MULTI-PHASE HIGH-TEMPERATURE ALLOYS (ORNL-2D)**
$110,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contacts:
M. P. Brady (865) 574-5153

The objective of this task is to develop high-strength, oxidation- and corrosion-resistant metallic and intermetallic alloys for use as hot components in advanced fossil energy conversion and combustion systems to help meet the efficiency and clean power generation goals of Vision 21. These alloys are needed to improve thermal efficiency through increased operating temperatures and decreased cooling requirements, as well as to provide materials for applications ranging from process monitoring (e.g. thermowells) to structural components or protective coatings in aggressive environments such as those encountered in coal gasification systems (e.g. molten salt, slag, ash, etc.). The development effort is based on increasing performance through fundamental understanding, manipulation, and control of multi-phase metallic (including intermetallic) structures.

Keywords: Alloys, Corrosion, Intermetallics

309. **DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES (ORNL-3B)**
$350,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact:
T. D. Burchell (865) 576-8595

The purpose of this work is to develop activated carbon molecular sieves (CMS) starting with porous Carbon Fiber Composites (CFC) manufactured from petroleum pitch derived carbon fibers. The Carbon Fiber Composite Molecular Sieves (CFCMS) will be utilized in Electrical Swing Adsorption (ESA) units for the efficient recovery separation of gases relevant to the fossil energy conversion process. With increasing interest in fuel cell technology and hydrogen as the preferred fuel for fuel cells, coal-derived synthesis gas has marvelous potential as a source of hydrogen. Oxygen-blown coal gasification is the most effective and efficient approach to achieving the goal of hydrogen from coal. Thus, a compact and efficient means of separating oxygen from air is being sought. A further purpose of this work is therefore to explore the utility of CFCMS/ESA for air separation.

Keywords: Activated Carbon, Composites

310. **CONTROLLED OXIDATION FOR FUNCTIONAL AND PROTECTIVE SURFACES (ORNL-4A)**
$150,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451

The goal of this program is to explore novel routes for controlling the chemistry and architecture of near-surface oxidation (nitridation, carburization, etc.) products that have application in advanced fossil-fuel fed systems by manipulating precursor alloy composition and microstructure. The effort will focus on gaining an understanding of the conditions under which the oxidation of multi-component, single-phase and multi-phase alloys can 1) controllably yield complex (ternary and higher order) ceramic phases in layered or dispersed (composite) arrangements of interest for functional applications (e.g., catalysts, gas sensors, etc.) and 2) establish continuous simple (binary) scales for protection in aggressive high-temperature environments, i.e., selective oxidation. The proposed program will primarily be based on studies of model systems selected from phenomenological as well as scientific considerations. However, a major aim of the program is to serve as an incubator for the spinoff of new processes and materials into applied development programs relevant to, and needed for, the building blocks of the Vision 21 power plant concepts.

Keywords: Alloys, Oxidation, Ceramics, Scales

311. **CRADA ON THERMIE ALLOY PROCESSING (ORNL-5M)**
$70,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Oak Ridge National Laboratory Contact:
R. W. Swindeman (865) 574-5108

The purpose of this task is cooperative work with Special Metals Corporation to develop the processing technology for Thermie alloy.

Keywords: Thermie Alloy, Processing

312. **DEVELOPMENT OF A COMMERCIAL PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS (REMAXCO-5)**
$125,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright
(865) 574-4451
ReMaxCo Technologies, Inc. Contact: R. D. Nixdorf
(865) 483-5060

MS&E has completed design of the new gas feed system and ReMaxCo is fabricating the system, RF Technologies has completed the design of the microwave feed system and reaction vessel. McCormick Engineering is completing the total furnace design. ReMaxCo has completed the fabrication of the MS&E gas feed system. RF Technologies is bench testing the microwave feed design. The reaction chamber vacuum vessel has been purchased. Bids for total system fabrication will be issued in April, 2004.

Keywords: Silicon Carbide, Microwave

313. **ALLUMINIDE COATINGS FOR POWER-GENERATION APPLICATIONS (TTU-2)**
$85,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Tennessee Technological University Contact:
Ying Zhang (931) 372-3186

The purpose of this task will be the fabrication, characterization and testing of aluminide coatings made on ferritic alloys such as Fe-9Cr-1Mo steels, which are being considered for use in advanced steam cycles. In addition, the influences of duty cycle length and operating temperature on the oxidation behavior of state-of-the-art bond coatings for fossil-fueled turbine engines are investigated.

Keywords: Aluminide, Coating, Steel, Power Generation

314. **MODELING OF CVD ZIRCONIA FOR THERMAL BARRIER AND ENVIRONMENTAL BARRIER COATINGS (UOL-1)**
$229,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Oak Ridge National Laboratory Contact: I. G. Wright
(865) 574-4451
University of Louisville Contact: T. L. Starr
(502) 852-1073

3-D modeling continues toward design of a sub-scale reactor to demonstrate rapid uniform deposition of thermal barrier coating on a full-width (12-cm) turbine blade section. At high deposition rate (>20 micron/hour) coating uniformity depends on uniform delivery of reactants to the blade surface. A practical reactor design likely will involve one or more small inlet nozzles impinging onto the blade surface. Previous model runs with a single 1cm inlet nozzle showed a parabolic deposition rate profile with ±30% variation over the full blade width. Model results for new designs with two and three nozzles show improved variability with ±10% variation in the central region of the blade. While the average deposition rate varies with temperature, reactant concentration and flow rate, the coating variability is related primarily to the geometry of the inlets—their location and spacing.

The above designs all involve steady-state reactor conditions with uniform reactant flows in all nozzles over the entire deposition period. A new approach involving variation of reactant flow rate over time is being evaluated. This would allow active control of coating uniformity during each turbine coating run.

Keywords: Coatings, Zirconia, Chemical Vapor Deposition

315. **Mo-Si ALLOY DEVELOPMENT (ORNL-2I)**
$150,000
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Oak Ridge National Laboratory Contact:
J. H. Schneibel (865) 574-4644

The objective of this task is to develop new generation corrosion resistant Mo-Si alloys for use as hot components in advanced fossil energy conversion and combustion systeMs. The successful development of Mo-Si alloys is expected to improve the thermal efficiency and performance of fossil energy conversion systems through increased operating temperatures, and to increase the service life of hot components exposed to corrosive environments at temperatures as high as 1600˚C. This effort thus contributes directly to Vision 21, one goal of which is to significantly reduce greenhouse emissions. The effort focuses presently on Mo-Si-B alloys containing high volume fractions of molybdenum silicides and borosilicides.

Keywords: Alloys, Molybdenum, Silicon

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

316. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS FOR STRUCTURAL AND FUNCTIONAL MATERIALS (ANL-1)**
$215,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 574-4451
Argonne National Laboratory Contact:
W. A. Ellingson (630) 252-5068

The work this period expanded on the two activities being addressed under this project. The two technical thrust areas are: 1) NDE technology development for thermal barrier coatings for advanced turbines, and 2) NDE technology development for characterizing high temperature gas-separation membranes.

Keywords: Non-Destructive Evaluation, Coatings, Membranes

317. **CORROSION AND MECHANICAL PROPERTIES OF MATERIALS IN COMBUSTION AND MIXED-GAS ENVIRONMENTS (ANL-4)**
$175,000
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Argonne National Laboratory Contact: K. Natesan
(630) 252-5103

Corrosion testing is continued on several Fe- and Ni-base alloys in the presence of coal-ash in support of advanced steam-cycle conditions. Experiments were completed at 725˚C. Two ash chemistries that included ash constituents, alkali sulfates and NaCl were used in the experiments. Several of the specimens, exposed at the three temperatures of 650˚, 725˚ and 800˚C, were mounted in metallographic mounts and polished. Optically examination of the specimens is continued.

Corrosion study was initiated in a steam environment at 725˚C with several Fe-base alloys that have been studied under simulated coal-slag environments. The alloys selected for the tests included HR3C, HR120, Save 25, NF709, modified 800, 347 stainless steel, HCM12A, Fe3Al clad 304, 671 clad 800H, and 310TaN. The specimens were exposed for 1850 h in an environment created by pumping water through a water pump and converting it to steam. The specimens were periodically retrieved after every 400 h and weight changes were measured. After 1850 h of exposure, small sections of the exposed specimens were cut for metallography examination and the remaining portions of the specimens were inserted for continued exposure. The cut pieces of the exposed specimens were mounted and polished for metallography. The oxide thickness and internal penetration in the substrate alloys were evaluated and the data are being analyzed.

Keywords: Alloys, Corrosion, Combustion

318. **IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS (FW-5)**
$80,000
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Oak Ridge National Laboratory Contact: I. G. Wright
(865) 574-4451
Foster Wheeler Development Corporation Contact:
J. L. Blough (201) 535-2355

The purpose of this project is to provide comprehensive corrosion data for selected advanced austenitic tube alloys in simulated coal ash environments. ORNL- modified alloys and standard comparison alloys have been examined. The variables affecting coal ash corrosion and the mechanisms governing oxide breakdown and corrosion penetration are being evaluated. Corrosion rates of the test alloys are determined as functions of temperature, ash composition, gas composition, and time.

Keywords: Alloys, Austenitic, Corrosion

319. **EFFECT OF CHROMIUM ON Fe/Al WELD OVERLAY COATINGS FOR CORROSION PROTECTION (LU-2)**
$100,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Oak Ridge National Laboratory Contact: I. G. Wright (865) 574-4451
Lehigh University Contact: J. N. DuPont and A. R. Marder (610) 758-4197

Several cast alloys representative of weldable Fe-Al-Cr weld overlay coating compositions were exposed to a Mixed Oxidizing/Sulfidizing Gaseous Environment (10%CO- 5%CO_2- 2%H_2O- 0.12%H_2S- N_2). The FeAlCr alloys (Fe-12.5Al, Fe-10Al-5Cr, and Fe-7.5Al-10Cr) were compared to a currently used Ni-based weld overlay coupon of Alloy 622. Samples were held at 500°C for 100 - 2000 hours. It was found that the corrosion kinetics for all three of the Fe-Al-Cr alloys were significantly lower than the corrosion kinetics of Alloy 622. For example, during 2000 hours of exposure to the corrosive environment, Alloy 622 gained approximately 20 mg/cm2 and all three of the FeAlCr alloys gained less than 0.5 mg/cm2 during 2000 hour exposure. Corrosion scale morphology was also considered and it was found that Alloy 622 formed a thick porous scale rich in nickel and sulfur, whereas the FeAlCr alloys formed small block-like nodules that were rich in iron and sulfur. It was concluded that several of the weldable FeAlCr overlay coating compositions could be deposited crack-free and can provide superior high-temperature corrosion protection to Alloy 622.

Weld overlay coatings were also characterized to determine if the weld microstructure had any effect on the cracking behavior of the welds. X-ray Diffraction (XRD) was used to identify the phases present within the weld overlay coatings. It was found that welds containing <6wt%Cr formed intermetallic phases (Fe3Al and/or FeAl) above approximately 11wt%Al. All alloys containing less than approximately 4wt%Cr formed (Fe,Al)3C carbides, which were identified using XRD. Alloys containing chromium additions greater than approximately 6wt%Cr showed only ferrite to be present, although weak Cr-rich carbide peaks were observed in these samples as well. Light Optical Microscopy (LOM) was also used to make observations about the weld microstructure. LOM observations of weld samples confirmed the existence of highly acicular carbides in welds containing lower chromium concentrations [(Fe,Al)3C] and small spherical carbides in samples containing high chromium concentrations [Cr-rich carbides]. The intermetallic phases cannot be observed using the LOM so the presence of this phase was not considered in the LOM observations.

Keywords: Coatings, Weld Overlay, Chromium, Alloys

320. **OXIDE DISPERSION STRENGTHENED (ODS) ALLOYS (ORNL-2E)**
$230,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
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The purpose of this task is to address the materials related barriers to expediting the use of oxide dispersion strengthened (ODS) alloys in components required in DOE's Office of Fossil Energy Vision 21 processes to operate at temperatures higher than are possible with conventionally strengthened alloys. Specific goals are to develop a detailed understanding of the behavior of ODS alloys in all phases of their use, including fabrication, service performance, life prediction, mode of failure, repair, and refurbishment. The scope of the effort includes the development of ODS iron aluminum alloys that combine strength levels of the same order as commercially available ODS FeCrAl alloys, with the superior resistance to high temperature sulfidation and carburization attack demonstrated by the best iron aluminides.

Keywords: Oxide Dispersion Strengthened (ODS), Alloys

321. **CONCEPTS FOR SMART PROTECTIVE HIGH-TEMPERATURE COATINGS (ORNL-4C)**

$70,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
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The overall purpose of this work is to assess the feasibility of different material and design approaches to smart protective coatings by exploring new alloying and microstructural approaches to improved high-temperature environmental resistance of metallic components.

Keywords: Coatings, Alloys, Microstructure, High-Temperature Protection

322. **DEFECT CONTENT IN ODS ALLOYS (UL-2)**
$100,000
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(865) 574-4451
The University of Liverpool Contact: A. R. Jones
151-794-8026

The purpose of this work is to assess the sources of defects in oxide-dispersion-strengthened (ODS) alloys. Experiments to confirm key features of defects in ODS alloys shall be devised and performed, and recommendations shall be made for the reduction of defects in these alloys.

Keywords: Oxide Dispersion Strengthened (ODS), Alloys, Defects

323. **MATERIALS TESTING IN FOSSIL ENERGY SYSTEMS (UNDEERC-4)**
$100,000
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(865) 576-4507
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(865) 574-4451
University of North Dakota Energy and
Environmental Research Center
(UNDEERC) Contact: J. P. Hurley
(701) 777-5159

The University of North Dakota Energy & Environmental Research Center (EERC) is providing expertise and assistance to Advanced Research Materials Programs investigating ceramic and alloy corrosion in fossil energy systeMs. It is difficult to simulate under controlled laboratory conditions all of the possible corrosion and erosion mechanisms to which a material may be exposed in an energy system. Therefore, the EERC is working with Oak Ridge National Laboratory (ORNL) to provide materials scientists with opportunities to expose materials in pilot-scale systems to conditions of corrosion and erosion similar to those occurring in commercial power systems.

The EERC has two pilot-scale solid fuel-fired systems available for exposure of material coupons. The slagging furnace system (SFS) is a high-temperature combustor built under the U.S. Department of Energy High-Performance Power System Program as a testing facility for advanced heat exchanger subsysteMs. In addition, a pilot-scale entrained-bed gasifier system known as the transport reactor development unit (TRDU) is available in which coupons can be exposed and hydrogen separation membranes tested under field conditions.

Keywords: Corrosion, Erosion, Testing

324. **INTEGRATED RESEARCH FOR PREDICTING HIGHER DIMENSIONAL PHASE DIAGRAMS WITH EMPHISIS ON TERNARY DIAGRAMS OF MOLYBDENUM (WVU-2)**
$60,000
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(865) 574-4451
West Virginia University Contact: Bruce S. Kang
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The aim of this research is to develop a predictive phase diagram ability, including the capability for predicting the ternary system formed by molybdenum, silicon, and boron.

Keywords: Molybdenum, Silicon, Boron, Phase Diagrams

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

325. **METALLIC FILTERS FOR HOT-GAS CLEANUP (AMES-3)**
$90,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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The objective of this study is to design and develop metallic filters having uniform, closely controlled porosity using a unique spherical powder processing and sintering technique. The corrosion resistance of the filter materials will be evaluated under simulated PFBC/IGCC gaseous environments in order to determine the optimum alloy composition and filter structure. The corrosion tests will also provide a means to estimate the service lives of experimental filter materials when subjected to either normal or abnormal PFBC/IGCC plant operating conditions. Metallic filters are expected to offer the benefits of non-brittle mechanical behavior and improved resistance to thermal fatigue compared to ceramic filter elements, thus improving filter reliability. Moreover, the binder-assisted powder processing and sintering techniques to be developed in this study will permit additional filter design capability (e.g., highly controlled filter porosity/permeability with greatly enhanced processing simplification), thus enabling more efficient and effective filtration.

Keywords: Filters, Hot-Gas Cleanup

326. **LOW-CHROME/CHROME-FREE REFRACTORIES FOR SLAGGING GASIFIERS (ARC-1)**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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Albany Research Center Contact: James Bennett
(541) 967-5873

High chrome oxide materials currently used as liners in coal and pet-coke slagging gasifiers have been found through experience to have the longest service life of any refractory material. The evaluation and development of refractory liner materials for slagging gasifiers has taken place over more than thirty years, with a minimum chrome oxide content of 75 pct thought necessary to achieve the best material performance. Even utilizing chrome oxide materials, refractory failure occurs in some locations of a gasifier in as short as 3 months, with other areas lasting no more than 18-24 months. Gasifier users would like a lining with a service life of at least 3 years. The primary causes limiting refractory service life are corrosion and spalling. Refractory failure by spalling is exasperated by frequent gasifier shutdowns related to other downstream issues. Refractory materials that do not contain chrome oxide or are low in chrome oxide are being considered as a replacement for high chrome oxide refractories for a number of reasons, including: 1) the high cost of chrome oxide refractories, 2) the potential for the formation of hexavalent chrome during service, an environmental carcinogen that may cause the spent refractory to be classified as a hazardous waste, 3) the difficulty in sintering high chrome oxide materials, and 4) the fact that high Cr2O3 refractories have not met the performance requirements of gasifiers. An increased understanding of high temperature material science, an increased understanding of how to design and use refractory materials in gasifiers, and better control and understanding of the gasifier and its operation should lead to improved non-chrome oxide/low chrome oxide refractories replacements for the Cr2O3 materials currently used in gasifiers.

Keywords: Refractories, Chrome-Free, Coat Gasification

327. **DEVELOPMENT OF CERAMIC MEMBRANES FOR HYDROGEN SEPARATION (ORNL-3B)**
$350,000
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Oak Ridge National Laboratory Contact:
R. R. Judkins (865) 574-4572

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, Coal Gasification

328. **EFFICIENT PRODUCTION OF HYDROGEN USING Pd MEMBRANE REACTORS (LANL-3)**
$100,000
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Steven A. Birdsell (505) 667-5868

Various diameters of porous stainless steel membrane were ion-milled and PVD coated with ~10 microns of V-7Cu alloy followed by a thin (100 nm) layer of palladium in order to obtain a hydrogen permeable composite membrane. Upon testing, the membranes still exhibited some porosity. A special PVD method is being developed to help seal the pores of the stainless steel membrane.

Keywords: Hydrogen, Membranes, Palladium

329. **MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS NEWSLETTER (MCNL-5)**
$60,000[22]
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Oak Ridge National Laboratory Contact: I. G. Wright
(865) 574-4451

The purpose of this task is to publish a bimonthly, joint DOE-EPRI newsletter to address current developments in materials and components in fossil energy applications.

Keywords: Fossil Energy, Newsletter

330. **HIGH-TEMPERATURE MATERIALS TESTING IN COAL COMBUSTION ENVIRONMENTS (NETL-4)**
$150,000
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National Energy Technology Laboratory Contact:
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Structural and functional materials used in solid- and liquid-fueled energy systems are subject to gas- and condensed-phase corrosion, and erosion by entrained particles. The material temperature and composition of the corrodents determine the corrosion rates, while gas flow conditions and particle aerodynamic diameters determine erosion rates for a given material. Corrodent composition depends on the composition of the fuel, the temperature of the

[22]Matching funding provided by EPRI.

material, and the size range of the particles being deposited. It is difficult to simulate under controlled laboratory conditions all of the possible corrosion and erosion mechanisms to which a material may be exposed in an energy system. Therefore, the University of North Dakota Energy & Environmental Research Center and the U.S. Department of Energy, National Energy Technology Laboratory are working with Oak Ridge National Laboratory to provide materials scientists with no-cost opportunities to expose materials in pilot-scale systems to conditions of corrosion and erosion similar to those in occurring in commercial power systems.

NETL is operating the Combustion and Environmental Research Facility (CERF). In recent years, the 0.5 MMBtu/hr CERF has served as a host for exposure of over 60 ceramic and alloy samples at ambient pressure as well as at 200 psig (for tubes). Samples have been inserted in five locations covering 1700-2600ºF, with exposures exceeding 1000 hours. In the present program, the higher priority metals are to be tested at 1500-1600ºF in one CERF location and near 1800-2000ºF at other locations to compare results with those from the EERC tests.

Keywords: Corrosion, Erosion, Coal Combustion

331. **ECONOMICAL FABRICATION OF MEMBRANE MATERIALS (ORNL-3H)**
$225,000
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The purpose of this task is to develop low-cost fabrication methods for asymmetric membranes which can be used for gas separation or catalysis. This project is focused on: 1) rapid sintering using focusing a focused infrared source and 2) deposition and characterization of ceramic membranes on porous metallic supports.

Keywords: Membranes, Low-Cost Fabrication

332. **MANAGEMENT OF THE ADVANCED RESEARCH MATERIALS PROGRAM (ORNL-5A)**
$400,000
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R. R. Judkins (865) 574-4572

The objective of the Advanced Research Materials Program is to conduct long-range research and development that addresses the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to provide technical management leadership for the DOE Fossil Energy Advanced Research Materials Program in accordance with procedures approved by DOE.

This task is responsible, in collaboration with DOE-HQ and DOE-NETL, for preparing planning documents, including R&D "road maps." ORNL is responsible for preparing its budget proposals (FWPs) for the program; recommending work to be accomplished by subcontractors, other federal laboratories, and by ORNL; placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; communicating program goals and results to industry and the research and development community; and reporting the progress of the program.

Keywords: Advanced Materials and Processing, Technical Management

333. **DEVELOPMENT OF SEALS FOR MEMBRANES (PNL-3)**
$450,000
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Oak Ridge National Laboratory Contact:
R. R. Judkins (865) 574-4572
Pacific Northwest National Laboratory Contact:
S. K. Weil (509) 375-6796

The purpose of this project is to develop the enabling sealing technology for high efficiency, low emissions fossil energy conversion, in support of the DOE-Office of Fossil Energy's Clean Coal Utilization and Vision 21 programs. Specifically, this project will focus developing the seals that are required to hermetically join inorganic membranes used in high temperature gas separation to the underlying support structure of the separation system. The seal materials must not only be compatible with both the: membrane and support materials, but must also be physically and chemically stable at the temperatures, pressures, gas atmospheres, and thermal cycling conditions typical of the electrochemical separation processes employed with gasified coal and air. The types of membrane materials that are being developed by the Office of Fossil Energy include microporous alumina and cerate-based perovskites for the separation of hydrogen from coal gas and syngas and transition metal oxide perovskites and brown millerites for the separation of oxygen from air. If successful, this project will aid in the deployment of these inorganic membranes to extract and utilize clean hydrogen from coal and will also establish the underlying technical basis required to evaluate the multiple approaches to inorganic membrane development that are currently being pursued.

Keywords: Membranes, Seals, Alumina, Perovskites

334. **PERSONAL SERVICES CONTRACT**
$20,000
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(865) 576-4507
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The task provides funds for a personal services subcontract for services related to the preparation of exhibits for and the management of exhibits at external conferences.

Keywords: Exhibits

335. **DEVELOPMENT OF ODS ALLOY FOR HEAT EXCHANGER TUBING (SMC-2)**
$160,000
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Oak Ridge National Laboratory Contact: I. G. Wright
(865) 574-4451
Special Metals Corporation Contact: Gaylord Smith
(304) 526-5057

This work is intended to generate information and understanding for incorporation into a database being generated by the team assembled by Special Metals Corporation to allow oxide dispersion-strengthened (ODS) alloys to be used in the design, construction, and operation of heat exchangers in the very high-temperature environments of interest in Vision 21 power plant modules. This effort has three main objectives: firstly, to characterize the effectiveness of modified processing routes aimed at optimizing the mechanical properties of the ODS-FeCrAl alloy INCO® MA956 for application as tubing. Property measurements from this activity will form part of the data package required for submission of a case for obtaining ASME Boiler and Pressure Vessel Code qualification for this alloy. Secondly, to evaluate the available techniques for joining ODS alloys, to provide a sound basis for fabrication options. The third objective is to develop a basis for service lifetime prediction based on the high-temperature oxidation behavior of this alloy.

Keywords: Oxide Dispersion Strengthened (ODS), Alloys, Heat Exchanger Tubing

336. **OPTIMIZATION OF ODS ALLOY PROPERTIES (UCSD-2)**
$100,000
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Long duration creep-life evaluation and stress-rupture testing is being performed on four creep-testing rigs (maximum test temperature = 1200°C) installed at UCSD during the course of this research program.

Test matrices are currently exploring threshold stress capabilities of transversely oriented specimens. Transverse creep specimens are extracted from as-extruded 1-3/8" OD tubes as follows: the tubes are split along their length by wire EDM, and then hot press-forged (single step) flat and/or rolled flat at 900°C. ASTM E-8 specimens are then spark machined from the forged piece. The machined test specimens are then subjected to a series of high temperature secondary recrystallization heat-treatments (over a range of time temperature combinations in different environments) prior to the incremental stress rupture tests. At the outset the bulk of the tests are conducted in air in the 900-1000°C temperature range.

Keywords: Oxide Disperson Strengthened (ODS), Alloys, Testing

337. **STUDY OF THE FATIGUE AND FRACTURE BEHAVIOR OF Cr-BASED ALLOYS AND INTERMETALLIC MATERIALS (UT-2A)**
$75,000
DOE Contacts: F. M. Glaser (301) 903-2784,
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(865) 974-6356

The TiAl intermetallic alloys with their low densities, improved oxidation resistances, good creep resistances, and high-temperature strengths made them very attractive materials for high-temperature applications. Efforts to enhance the ductility, and refine the grain size in these materials have focused on the addition of alloying elements. The addition of Nb provides the most effective method for improving the room-temperature ductilities, fracture toughnesses, and oxidation resistances. The addition of W can result in an enhancement of mechanical properties, such as yield strengths, ultimate tensile strengths, and the refinements in microstructures. The boron addition in lamellar TiAl alloys has a significant effect on room-temperature tensile ductilities.

Keywords: Intermetallics, Chromium, Alloys, Fatigue, Fracture

ULTRA-SUPERCRITICAL STEAM POWER PLANT RESEARCH

338. **ULTRA-SUPERCRITICAL STEAM TURBINE MATERIALS (ARC-2)**
$200,000
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Albany Research Center Contact:
Richard P. Walters (541) 967-5873

This research will provide the base materials technology needed to design steam turbines capable of operating at temperatures and pressures typical of ultra-supercritical steam conditions. The tasks to be undertaken include: 1) a detailed review of the current technology; 2) the identification of the critical issues and major barriers in relation to the target high pressure (HP), intermediate pressure (IP), and low pressure (LP) steam condition; 3) the identification of promising materials and a plan to evaluate and qualify materials for the critical components; and 4) the recommendation of materials constitutive equations, damage evaluation criteria, and life-prediction criteria that would be needed for a proof-of-concept design and analysis.

Keywords: Steam Turbine, Ultra-Supercritical

339. **MATERIALS FOR ULTRA-SUPERCRITICAL STEAM POWER PLANTS (FEAA061)**
$1,020,000
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This research is part of eight tasks undertaken by a consortium of utilities, boiler manufacturers, materials producers, the Electric Power Research Institute, the State of Ohio, and the U.S. Department of Energy which are directed toward resolving the major materials issues confronting the ultra-supercritical coal power plant. These tasks include 1) conceptual design and economic analysis, 2) mechanical properties of advanced alloys, 3) steam-side oxidation evaluations, 4) fireside corrosion evaluations, 5) welding development, 6) fabrication development, 7) coating development, and 8) design methodology. The achievement of the goals of this program will produce the capability to construct and operate a boiler to steam conditions of 760˚C (1400˚F) and 35 MPa (5000 psig).

Keywords: Ultra-Supercritical, Alloys, Oxidation, Corrosion, Welding, Coating, Fabrication

340. **ULTRA-SUPERCRITICAL STEAM CYCLE TURBINE MATERIALS (FEAA069)**
$350,000
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This research will provide the base materials technology needed to design steam turbines capable of operating at temperatures and pressures typical of ultra-supercritical steam conditions. The tasks to be undertaken include: 1) a detailed review of the current technology; 2) the identification of the critical issues and major barriers in relation to the target high pressure (HP), intermediate pressure (IP), and low pressure (LP) steam condition; 3) the identification of promising materials and a plan to evaluate and qualify materials for the critical components; and 4) the recommendation of materials constitutive equations, damage evaluation criteria, and life-prediction criteria that would be needed for a proof-of-concept design and analysis.

Keywords: Ultra-Supercritical, Steam Turbine, Constitutive Equations, Life-Prediction

ADVANCED METALLURGICAL PROCESSES PROGRAM

The materials program at the Albany Research Center (ARC) incorporates Advanced Metallurgical Processes that provide essential life-cycle information for evaluation and development of materials. The research at ARC directly contributes to FE objectives by providing information on the performance characteristics of materials being specified for the current generation of power systems, on the development of cost-effective materials for inclusion in the next generation of fossil fired power systems, and for solving environmental emission problems related to fossil fired energy systeMs. The program at ARC stresses full participation with industry through partnerships and emphasizes cost sharing to the fullest extent possible.

The materials research in the Program focuses on extending component service lifetimes through the improvement and protection of current materials, by the design of new materials, and by defining the service operating conditions for new materials in order to ensure their safe and effective use. This process involves developing a better understanding of specific failure modes for materials in severe operating environments, addressing factors which limit their current use in these environments, and by designing new materials and materials processing procedures to overcome anticipated usage challenges in severe operating environments, such as those typically found in fossil energy generating plants and in structures and supporting facilities associated with oil and gas production. Emphasis is placed on high-temperature erosion testing and modeling in environments anticipated for FutureGen programs, development of casting technologies and new alloys to improve wear resistance in those environments, on development of sulfidation/oxidation resistant materials which can also resist thermal cycling for pressurized circulating fluidized bed reactors, and on repair and development of refractory materials for coal gasifiers. DOE contact is Alan D. Hartman (541) 967-5862.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

341. **ADVANCED FOIL LAMINATION TECHNOLOGY**
$600,000
DOE Contact: Alan D. Hartman (541) 967-5862
Albany Research Center Contact: Arthur V. Petty, Jr. (541) 967-5878

ARC researchers have developed a materials fabrication approach that utilizes dissimilar foils to produce a variety of materials (e.g., layered composites, monolithic metallic and intermetallic alloys). The research has identified bonding parameters for laminating type 347-stainless steel foils. This technique has also been used to join dissimilar metals. The goal of this research is to use conventional deformation processing techniques (such as extrusion or rolling) to bond foils to substrates and to each other.

Keywords: Aluminides, Coatings, Foil-Lamination Process

342. **ADVANCED CASTING TECHNOLOGIES**
$301,000
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Most wear-resistant components are produced using metal casting technologies. ARC has developed expertise in recent advanced casting technologies, which may be applied to production of components for fossil energy plants. The goal of the research is to understand the mechanisms of current component degradation and to produce new alloys via casting for increased service life and power plant operational efficiency.

Keywords: Alloys, Casting

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

343. **ADVANCED REFRACTORIES FOR GASIFIERS**
$900,000
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Albany Research Center Contact: Arthur V. Petty, Jr. (541) 967-5878

The emphasis of this high temperature material research has been driven by both short-range industrial needs and long-range issues in gasifiers. Program emphasis is on: 1 identifying material failure mechanisms 2) identifying/ developing materials that will extend the lifetime of primary refractory liners in slagging gasifier systems 3) developing repair techniques to shorten system downtime caused by refractory maintenance, and 4) developing improved thermocouples/temperature-monitoring techniques. A refractory material with improved resistance to attack by molten coal slags in simulated gasifier environments has been developed.

Keywords: Refractories, Slagging Gasifier, Liners, Thermocouples

344. **OXIDATION AND SULFIDATION RESISTANT MATERIALS**
$600,000
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Albany Research Center Contacts:
Arthur V. Petty, Jr. (541) 967-5878 and
Cindy Doğan (541) 967-5803

The goal of this research is to develop modified austenitic stainless steels with performance characteristics necessary for process streams in advanced heat recovery and hot gas cleanup systems employed with advanced power generation systems (IGCC, PFBC and IGFC). The most difficult near term R&D challenges are development of hot gas particulate and sulfur cleanup systems employed with these advanced power generation systeMs. Primary focus is on the development of TiC-reinforced *cast* austenitic stainless steels with Al and Si additions for oxidation and sulfidation resistance.

Keywords: Alloys, Casting, Cast Austenitic Stainless Steel, Titanium Carbide

345. **WEAR AND ABRASION OF MATERIALS FOR FOSSIL ENERGY SYSTEMS**
$600,000
DOE Contact: Alan D. Hartman (541) 967-5862
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Wear and erosion are significant materials-related problems found in the operation of fossil energy plants. By understanding the general wear and erosion mechanisms that occur in coal preparation and plant operation, materials and procedures can be developed to reduce the effects of these mechanisMs. A better understanding of micro-mechanisms of material removal is needed, as well as a basic understanding of the mechanics of deformation during erosion. The project investigates preparation of non-conventional materials and their performance under simulated pulverized coal combustion plant conditions. Improvements will result in higher efficiency, less maintenance and fewer catastrophic failures in fossil energy plants. An understanding of material behavior under conditions of impact by dry particles will be developed along the way, through understanding the contact mechanics of the impact process and by investigating and characterizing the damage inflicted on various materials by impact of particles.

Keywords: Abrasion, Erosion, Oxidation, Corrosion, Wear

346. **MECHANISMS OF CORROSION UNDER ASH DEPOSITS**
$750,000
DOE Contact: Alan D. Hartman (541) 967-5862
Albany Research Center Contact: Cindy Doğan (541) 967-5803

The focus of the project is understanding the effect of ash deposits on the corrosion of metals and alloys, and developing recommendations for improved alloys or operating conditions to reduce the level of corrosion. Three power generation industries (coal combustion, coal gasification, and waste incineration) share the problem of accelerated corrosion of metallic components due to ash deposition. While ash composition is different for each of these industries, all of the ash deposits tend to absorb impurities from the gaseous atmosphere, keeping them near the metal surface where the corrosion reaction occurs.

Keywords: Corrosion, Molten Salts, Hot Corrosion

347. **NON-ISOTHERMAL CORROSION AND OXIDATION**
$300,000
DOE Contact: Alan D. Hartman (541) 967-5862
Albany Research Center Contact: Cindy Doğan (541) 967-5803

Large temperature gradients and heat fluxes occur in turbines, heat exchangers, and walls of fossil energy power plants. The objective of this research is to determine the effects of thermal gradients and heat fluxes on oxidation, sulfidation, and hot corrosion behavior of metals commonly used in high-temperature components of fossil energy power plants. A thermal cycling test facility will examine non-isothermal oxidation and hot corrosion.

Keywords: Oxidation, Corrosion, Thermal Gradient

348. **CORROSION RESISTANT NEW MATERIALS FOR SOLID OXIDE FUEL CELL INTERCONNECTS**
$350,000
DOE Contact: Alan D. Hartman (541) 967-5862
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The chief characteristic of fuel cells is the ability to convert chemical energy to electrical energy without the need for combustion, giving much higher conversion efficiencies than conventional methods. Costs of fuel cells remain an issue and can be reduced in component fabrication, materials used, and cell and stack designs. Projections indicate that by replacing currently used ceramic interconnects with metallic interconnects could reduce materials costs by approximately 85 percent. The objective of this research is to determine applicability of new corrosion-resistant alloys for use as metallic interconnects through studying the alloy corrosion behavior in simulated and real solid oxide fuel cell environments which can approach 1000°C.

Keywords: Oxidation, Corrosion, Fuel Cells

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INDEX

A

Ab-Initio (146)
Ablator (150, 151)
Abrasion (166)
Abrasive Wear (64)
Absorption (147)
Actinides (125)
Activated Carbon (156)
Active Control (140)
Adhesion (143)
Adhesive Bonding (24)
Advanced Composite Materials (64)
Advanced Computational Techniques (67)
Advanced Heat Engines (19)
Advanced Insulation (16)
Advanced Materials (34, 64, 69)
Advanced Materials and Processing (162)
Advanced Packaging (148)
Advanced Processes (34, 48, 51)
Aerogels (16, 64)
Aftertreatment (21)
Aging (40, 142, 149)
Air Purging (79)
Alanates (39, 40)
Algorithms (149)
Alloys (19, 35, 51-54, 65-67, 69, 120, 154, 156-160, 163-165)
Alumina (48, 49, 162)
Alumina Crucible Cell (47)
Alumina Electrolysis Cells (53)
Aluminides (155, 157, 165)
Aluminosilicate (66)
Aluminum (22-24, 32-34,50, 51, 54, 57, 66, 80, 82)
Aluminum Carbothermic Reduction (48)
Aluminum Castings (82)
Aluminum Conductors (78)
Aluminum Ingot (54)
Aluminum Iron Alloys (83)
Aluminum Melting (48, 53)
Aluminum Potroom Operation (47)
Aluminum Production (47, 83, 84)
Aluminum Products (79)
Aluminum Reduction (47, 79)
Aluminum Refining (47)
Aluminum Scrap (54)
Aluminum Smelting (82)
Aluminum Strip and Sheet (54)
Ammonia Refrigeration (79)
Amorphous Materials (72)
Amorphous Silicon (72)
Analytical Microscopy (73)
Anistropic Magnets (107)
Annealing (50, 54)
Anodes (51, 82- 84)
Assessment (23)
Assessments (35)
ASTM (33)
Atomic Force Microscopy (150)
Atomic-Level (142)
Austenitic (159)
Austenitic Stainless Steel (30)
Auto Manufacturing (80)
Automation (59)
Automotive (19, 22, 25, 33)

B

Back-Surface Field (74)
Beryllium (150)
(Bh)max (107)
Billet (69)
Bioactive Materials (140)
Biomemetics (73)
Biomineralization (150)
Biomolecules (138)
Bipolar Plates (41)
Birefringent (137)
Bismuth Conductor (92)
Bonded Magnets (107)
Bonding (63)
Borides (47, 64, 160)
Boundary Lubrication (80)
Brakes (23, 34)
Brazing (82, 135)
Buffer Layers (90)
Building Materials (15)
Buses (33)

C

Cables (80)
Cadmium Telluride (72)
Calcination (125)
Calibration (58)
Carbide Derived Carbon (69)
Carbon (19, 41, 42)
Carbon Materials (20, 34, 40, 6, 1289)
Carbon Monolith (34)
Carbon Nanotubes (40)
Carbon Particulates (21)
Carbon-Fiber Reinforced Polymer Matrix Composites (23)
Carbothermal Reduction (31)
Carburization (67)
Cast Aluminum Parts (85)
Cast Austenitic Stainless Steel (165)
Cast Metals (22, 57, 58)
Casting (23, 33, 52-54, 58, 66, 165)
Casting Optimization (82)
Catalysts (27, 65, 83, 139)
Cathode (51, 82)

Cements (37)
Ceramics (21, 22, 29, 35, 37, 53, 63, 64, 66, 69, 77, 79, 83, 123, 135, 141, 155, 157, 161)
Cermets (22, 25, 26, 28)
CFC (14)
CGI Castings (81)
Characterization (70)
Chemical Analysis (145, 149)
Chemical Specificity (147)
Chemical Vapor Deposition (63, 72, 108, 157)
Chemical Vapor Infiltration (64)
Chemiresistance (136)
Chlorine (49)
Chrome-Free (161)
Chromium (159, 164)
Chromium-Free (59)
Chromophore (145)
CIDI (22)
Clad Vent Sets (128)
Clathrate-Like (146)
Cleanliness Analysis (59)
Coal Combustion (162)
Coal Gasification (161)
Coated Conductor (90)
Coatings (21, 41, 63, 64, 66, 68, 69, 78, 120, 154-157, 159, 164, 165)
Coatings and Films (72)
Coking (69)
Collective Phenomena (147)
Colloids (143)
Combinatorial (67)
Combustion (156, 158)
Compatibility (120, 129)
Complex Hydrides (39, 40)
Components (35)
Composites (35, 64, 80, 82, 121, 131, 155, 156)
Computational Fluid Dynamics (59)
Concentrator Cells (73)
Concrete (126)
Conductive Polymers (73)
Connecting Rods (23)
Constitutive Equations (164)
Constitutive Models (60)
Contact Damage (32)
Contamination (126)
Continuous Casting (50)
Coolant Behavior (55)
Coordinate Measurement Machine (81)
Coordination (19)
Copper Indium Diselenide (72)
Copper Motor Rotors (84)
Corrosion (31, 37, 41, 56, 63, 64, 67, 69, 79, 126, 131, 142, 144, 145, 155, 156, 158-160, 162, 164, 166)
Cost (23, 35)
COTS (145)
Crashworthiness (23)
Creep (32, 56, 65, 69)
Cryolite (48, 52)
Crystal Growth (150)
Crystalline Defects (74)
Crystalline Silicon (72, 74)
Crystallization (65)
Cupola Furnace (81)
Current Limiter (91)

D

Decontamination (139)
Deep Ultraviolet Lithography (108)
Defects (160)
Degassing (54, 66)
Degradation (141, 142, 144)
Delocalization (145)
Deposition (90)
Diamond Composites (65)
Die Casting (22, 24, 56, 58, 68, 77, 80, 84)
Diels-Alder (139)
Diesel (21, 22, 27, 82)
Diesel Exhaust (22)
Differential Scanning Calorimetry (67)
Diffraction Grating (124)
Dilatometry (61, 67)
Dip-Pen Nanolithography (150)
Direct Chill Casting (50, 54, 55)
Dislocations (143)
Dispersion Strengthening (69)
Dissimilar Materials (23, 34)
Drilling (30)
Dross (48)
Ductility (30, 64, 81)
Duplex Stainless Steel (58)
Durability (23, 24)
Dynamic Windows (15)

E

Eddy-Current (81)
EDM (30)
EGR (31)
Electro-Optics (140)
Electrochemical Cell (68)
Electrochemical Sensor (22)
Electrochromic (15)
Electrodeposition (72, 137, 142)
Electrodes (83)
Electroless (85)
Electrolytic Cells (49)
Electrolytic Reduction (52)
Electrolytic Tin Plate (59)
Electromagnetic Forming (22)
Electrometallurgical (49)
Electron Beam Welding (86)
Electron Microscopy (74, 149)
Electroplating (135, 148)
Electrowinning (82)
Emissions (52)
Encapsulants (134, 141)

Energetic Materials (149)
Energy Storage (81)
Erosion (160, 162, 166)
Ethylene (69)
Ethylene Production (83)
EUV (149)
Exhaust Aftertreatment (26)
Exhaust Emissions (27)
Exhaust System (30)
Exhibits (163)
Extrusion (22, 33, 52, 69, 128)

F

Fabrication (164)
Failure Analysis (21)
Fatigue (61, 69, 164)
Ferritic Steel (65, 130, 131)
Ferroelectric (141)
Ferromagnetism (65)
Ferrous Alloys (65)
Fiber Preforming (24)
Fiber Reinforcement (37)
Fibrous Materials (64)
Field Structuring, Composites (136)
Film Silicon (72)
Filters (21, 160)
Finite Element Modeling (69)
First-Principles Modeling (143)
Flexural Strength (33)
Fluidized Bed Furnace (85)
Flux Pinning (92)
Flywheel (91)
Foam Insulation (14)
Foamed Metals (34)
Foams (62, 134)
Focal Project Design (25)
Focused Ion Beam (148)
Foil (154, 165)
Forging (68, 81)
Forming (24, 33, 53, 61)
Fossil Energy (161)
Foundry Sand (81)
Fourier Transform Spectroscopy (74)
Fracture (33, 53, 64-66, 164)
Frames (33)
Frequency-Selective Glass (78)
Friction (29, 34, 69)
Fuel Cells (28, 41, 166)
Fuel Injectors (21, 22)
Fuel Processing (42)
Fuel Systems (25, 26)
Functional Assemblies (138)
Functional Materials (140)
Furnace (56, 69, 83)
Fusion Zone (136)

G

Gallium Arsenide (73)
Galvanized Steel (23)
Gamma Radiolysis Experiments (129)
Gas Fluxing (49)
Gas Turbines (78)
Gasochromic (15)
Gelcasting (21, 22)
Generator (91)
Geologic Repository (122)
Geothermal Piping (37)
Geothermal Wells (37)
Germanium Compounds (83)
Gettering (134, 147)
Glass (56, 67, 68, 79,82, 84, 123, 125)
Glazing (24, 78)
Gleeble (61)
Grain Refinement (66)
Grain Size (65)
Grain-Boundary (142)
Gray Iron (58)
Grinding (30)
Guided Waves (37)

H

Hall-Héroult Process (52)
Hamiltonians (143)
HCFC (14)
Heat Checking (58)
Heat Exchange Method (HEM) (74)
Heat Exchanger (34, 41, 163)
Heat Sinks (20)
Heat Transfer (20, 131)
Heat Treating (66, 68, 85)
Heat-Air-Moisture (15)
Heavy Vehicle (34)
Helium Embrittlement (130)
High Density Infrared Heating Technology (63)
High Pressure Techniques (65)
High Rate Processing (25)
High Strain Rate (142)
High Strength Steel (24)
High Temperature (56, 67, 78, 128)
High Volume Processing (24)
High-Efficiency Silicon Cell (74)
High-Efficiency Solar Cells (73)
High-Level Waste (125)
High-Speed Imaging Techniques (107)
High-Strength Steels (60-62)
High-Temperature Components (156)
High-Temperature Protection (159)
Hot Corrosion (166)
Hot Dip Processing (59)
Hot Rolling (50, 51)
Hot Strip Mill (61)

Hot-Gas Cleanup (160)
HotEyeTM (81)
Hydrocarbon Fluorination (83)
Hydroceramic (125)
Hydroforming (22)
Hydrogen (39, 40, 74, 131, 135, 139, 161)
Hygrothermal (15)
Hyperspectral Image (144)

I

Ice-Like (146)
IEA (32, 33)
III-V Material (73)
Immersion Heater (55)
Inclusions (58-61)
Industrial Boilers (68)
Industrial Chemicals (69)
Industry (70)
Inert Anodes (47, 53)
Infrared (32, 64, 66)
Infrastructure (23)
Ingot Casting (51)
Ink-Jet Printing (136)
Inserts (58)
Inspection (30)
Insulation Sheathing (14)
Insulation/Thermal (128)
Interfaces (147)
Intermetallics (25, 26, 156, 164)
Investment Casting (84)
Ion Exchanger (123)
Ionic Fluids (15, 52)
IR (64, 149)
Iridium Alloy (129)
Iridium Processing (128)
Iron Phosphate Glasses (84, 123)
Ironmaking (62)
Irradiation (120, 121, 130)
Isothermal Melting Process (55)

J

Joining (23, 70)

L

Lamellar Microstructure (30)
Langmuir Probe (142)
Laser Fusion Targets (150, 151)
Laser Surface Texturing (31)
Laser Welding (136)
Laser/Material Interaction (136)
Lead Bismuth (130)
LED (79)
LED-Activated Lamps (79)
Life Prediction (21, 27, 29, 164)
Lifetime (59, 142)
LIGA (137, 148)
Light Trapping (74)
Lightweight (33)
Lightweight Alloys (33)
Liners (165)
Liquid-Phase Epitaxy (73)
Lithium (120)
Lithography (135)
Lost Foam Casting (57, 82, 85)
Low Cost Carbon Fiber (24)
Low-Cost Fabrication (162)
Low-Cycle Fatigue (32)
Low-Dross Combustion (49)
LST (31)

M

Machining (30, 57, 58)
Magnesia (66)
Magnesium (22, 24, 33, 34, 81, 85)
Magnetic Resonance (91)
Magnetism (65, 83, 142, 149)
Magnetohydrodynamic (51)
Magnetoresistance (136)
Magnetostriction (149)
Management (19)
Manufacturing (25, 33, 135)
Materials (33, 35, 37, 67, 70, 78, 139, 145, 146)
MBE (73, 74)
MEA (40)
Mechanical (29, 37, 64, 142)
Mechanical Properties (21, 63-65, 129)
Melting (52, 128, 136)
Membranes (68, 161, 162)
MEMS (136, 145, 148)
Mesabi Nugget Project (62)
Mesoporous (64, 139)
Metallic Anode (79)
Metallic Phases (65)
Metals (19, 23, 50, 56-58, 66, 69, 70, 77, 80, 85, 126, 135, 139, 143)
Microdevices (137, 147)
Microelectronics (140, 144, 145)
Microfabrication (135)
Microfluidics (140)
Micromachining (108, 137, 147)
Microporous Materials (48)
Microscale Welding (148)
Microscopy (143)
Microstructure (27, 40, 53, 54, 58, 65, 66, 135, 142, 146, 155, 159)
Microsystem (142)
Microtexture (50)
Microwave (21, 24, 49, 157)
Milling (30)

Minority Carrier Lifetime Measurement (73)
Mmc (34)
MMC Material (82)
MOCVD (73, 74)
Modeling (56, 58, 59, 61, 65, 69, 70, 121, 126, 130, 142)
Module Testing (73)
Moisture (15)
Molds (52, 68)
Molten Glasses (125)
Molten Salts (131, 166)
Molybdenum (154, 158, 160)
Monitor (56)
Monolayer (146)
Monolithics (64, 66)
Motor (91)
Motor Brushes (80)
Multi-Layered-Surface Coatings (56)
Multicrystalline Silicon (74)
Multilayer/Nano-Laminate Technology (149)
Multivariate Analysis (149)
Multivariate Calibration (144)

N

Nano Materials (28)
Nanocrystalline (73, 146)
Nanolayers (137)
Nanolithography (145)
Nanomaterial (143, 145)
Nanoparticles (138, 139)
Nanoporous (64)
Nanoscale (141, 150)
Nanostructure (65, 73, 74, 136, 138, 146)
Nanowires (138)
Natural Gas Storage (34)
NDE (23, 29)
NdFeB (20)
Near Frictionless Carbon (69)
Near-Field (122)
Net Shape (85)
Newsletter (161)
NEXAFS (141)
Next-Generation Photovoltaics (73)
NiAl (26)
Nickel Alloy Substrate (107)
Nickel Aluminide (31)
Nickel Plating (85)
Nickel-Based Superalloy (79)
Niobate (123)
Nitride (41)
NMR (141)
Non-Destructive Testing (29, 37, 73)
Non-Equilibrium Microstructures (148)
Non-Vacuum (86)
Nonthermal Plasma (21)
NO_x (22, 26, 27)
Nozzles (21)
Nuclear Waste (123)
Nucleation Density (108)
Numerical Modeling (23, 69)

O

Operations Control (81)
Optic Systems (149)
Optoelectronics (140)
Ordering in Semiconductors (74)
Organic Solar Cells (73)
Orifice (21)
Oxidation (52, 157, 164, 166)
Oxide Buffers (107)
Oxide Dispersion Strengthened (ODS) (159, 160, 163)
Oxide Sludge (48)
Oxy-Fuel (56)
Oxygen Consuming Cathode (68)

P

Packaging (145, 147)
Palladium (161)
Paramagnetism (65)
Particle Size (124)
Particulate Emissions (27)
Passivation (59, 142)
Passive Electonic Devices (149)
Passive Heating (15)
Permanent Magnets (20, 107)
Permanent Mold Casting (84)
Permeability (149)
Perovskites (162)
Phase Change (15)
Phase Diagrams (160)
Phase Equilibria (65, 125)
Phosphors (79)
Photo-Active (139)
Photochromic (137)
Photoelectrochemical Materials (74)
Photonics (137, 140, 141)
Photoresist, Micro-Gravity (141)
Photosensitive (137)
Photovoltaic (78)
Physical Vapor Deposition (72)
Piezoelectric Actuators (25)
Piezoresistance (136)
Planning (35)
Plant Reliability (37)
Plasma Plume (142)
Plasma Polymer (151)
Plasma Processing (63)
Plasma Spraying (28)
Plasma-Facing Materials (121)
Plastic Deformation (55)
Point Defects (74)
Polycrystalline Films (72)
Polyimide (150)

Polymers (23-25, 34, 73, 134, 137, 150, 151)
Porosity (57, 66)
Pot Hardware (59)
Potlining (47)
Powder Metallurgy (31, 62, 83)
Powder Synthesis (31)
Power Electronics (20, 21)
Power Generation (157)
Precision Thin Films (149)
Precursors (24)
Primary Aluminum (48, 49, 52)
Processing (24, 64, 70, 77, 155, 157)
Properties (15, 56, 70)
Pulsed Laser Deposition (64)
Pumps (23)
PV Systems (81)
Pyramid Molds (108)
Pyrolysis (63)

Q

Quantum Mechanical (147)
Quaternary Semiconductors (73, 74)
Quench Wheel (107)

R

Rabits (107)
Radiation (122, 123, 141)
Radiator (41)
Radio Frequency Magnetron Sputtering (107)
Radioactive Waste (124)
Radionuclides (126)
Rapid Prototyping (24)
Rapid Solidification (68, 107)
Rapid Thermal Processing (72, 74)
Rapid Tooling (56)
Recrystallization (50)
Recycle (24)
Refractories (55, 56, 64, 66, 67, 78, 83, 121, 129, 161, 165)
Refrigerators (14)
Reinforcement (57)
Reliability (141)
Resistance Welding Electrode (80)
Reverberatory Furnaces (49, 53)
Rheology (137)
Rolling (52)
Rolling Contact Fatigue (32)
Roofs (14)
Rotating Equipment (62, 69, 78)

S

Salt Eutectics (82)
Salt Fluxing (52)
Sand Casting (58, 85)
Scales (157)
SCR (26)
Scrap Reduction (85)
Screen Printing Metallization (74)
Scuffing (29)
Seals (162)
Secondary Aluminum (49)
Self Assembly (136)
Semi-Solid Molding (85)
Semiconductors (72-74, 108, 141)
Sensors (26, 53, 134, 136, 149)
Separations (68, 91)
Sheet Forming (22)
Shock Response (141)
Silica-Based Glass Fibers (84)
Silicon (72, 74, 108, 121, 154, 157, 158, 160)
Silicon Carbide (SiC) (65, 69, 83,122)
Silicotitanate (123)
Simulation (22, 121)
Sintering (66, 135, 141)
Slagging Gasifier (165)
Slurry (124)
Smelting (47, 51)
SO_2 (85)
Sodium-Bearing Waste (125)
Soft Solution Processes (143)
Sol-Gel (64, 68)
Solar Cells (72-74, 78)
Solar Concentrators (78)
Solar Control (15)
Solar Heat Gain Coefficient (15)
Soldering (135)
Solid State Spectroscopy (74)
Solid Waste Recycling (77)
Solvents (65)
Spatter (136)
Spectroscopy (124, 125, 149)
Spin Coating (141)
Spot Welding (24, 62, 82)
Spray Forming (54, 68)
Sputtering (72, 150)
Squeeze Casting (57)
Stainless Steel (65)
Stamping (24)
Standards (33)
Steam Turbine (164)
Steel (33, 57, 59-62, 66, 85, 86, 121, 157)
Strain and Water Chemistry (68)
Strain Rate (23, 60)
Stress Assisted Corrosion (68)
Stress-Strain Behavior (61)
Structural Analysis (37)
Structural Materials (18, 24, 34, 130, 149)

Sulfidation (145)
Sulfur Removal (42)
Superconductor (20, 90, 92)
Superhard Materials (65)
Superlattices (137)
Superplastic Forming (33)
Supersaturation (138)
Surface Characterization (73, 50, 56, 86, 145)
Surface Interactions (147)
Surface Treatment (32)
Surfactants (139)
SXR and XR Optics (149)
Synthetic Lumber (77)

T

Ta-10w Oxidation (129)
Technical Management (23, 35, 162)
TEM (27)
Temperature Measurement (30)
Templates (138, 150)
Tensile Strength (65, 66)
Ternary Semiconductors (73)
Testing (160, 163)
Textured Substrate (90)
Thermal Management (20, 41)
Thermal Properties (22, 28, 33, 63, 129, 166)
Thermal Spray (63, 135)
Thermal Storage (15)
Thermie Alloy (157)
Thermochemical (67)
Thermocouples (165)
Thermodynamic (52, 65, 139)
Thermomechanical Processing (51, 58)
Thermophysical Properties (67)
Thermoresistance (136)
Thin Films (28)
TiC (26)
Tiles (15)
Time-Dependent (142)
Titanium (30, 31, 34, 80, 165)
Tool Steel (68)
Traction Motors (20)
Transformation (61, 65)
Transient Liquid Coatings (63)
Transmission and Distribution Lines (78)
Transmission Cable (91)
Transmission Electron Microscopy (40)
Transmutation (130)
Transport (126)
Trap Materials (27)
Tribology (28, 29, 52, 137, 142, 147)
Trifluoroacetate Solution Process (107)
Trucks (33)
TTBC (28)
Tubes (66, 68, 69)
Tungsten Carbide (80)
Turbine Blades (79)
Turning (30)

U

Ultra-Supercritical (164)
Ultrafine Grained Material (55)
Ultrananocrystalline Diamond (63)
Ultrasonics (34, 37, 54, 66, 124)
User Center (70)
UV (64, 149)

V

Vacuum Arc Melting (66)
Vacuum-Arc Plasmas (142)
Valves (27)
Vanadium (86, 120)
Variability (60)
Viscosity (124)
Visible (149)
Vitrification (123)
Voltage (47)

W

Waste Reduction (85)
Waste Utilization (85)
Water (146)
Wear (28, 63, 64, 166)
Wear Reduction (80)
Wear Resistance (80, 86)
Weld Overlay (159)
Welding (24, 65, 69, 70, 77, 135, 164)
Windows (78)
Workshops (35)

X

X-ray (135)
X-ray Absorption (125)

Z

Zeolites (68, 124, 125)
Zinc Alloys (56)
Zinc Die Casting (56)
Zirconia (157)
ZnO (138)