DOE/SC-0077

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 2002

August 8, 2003

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

PROGRAM DESCRIPTIONS

TABLE OF CONTENTS (continued)

LIST OF TABLES

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. The EMaCC Charter and the memorandum approving it are presented in the Appendix of this report.

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 4-6.

Four meetings were scheduled for 2002-2003. The dates and minutes from the meetings are as follows:

OCTOBER 17, 2002, GERMANTOWN

Chairman, Dr. Udaya Rao, opened the meeting by having the participants introduce themselves.

Robert Gottschall (BES) presented the format and expected outcome of the Workshop on *Basic Research Needs to Assure a Secure Energy Future*. This workshop was held October 21-25, 2002, by a sub-panel of the Basic Energy Sciences Advisory Committee (BESAC). The outcome of the workshop is to be a list of proposed research directions and supporting statement for each entry (including impact and time scale) that BESAC as a whole will consider. A preliminary presentation will be made to BESAC at its November 5-6, 2002, meeting. The full report will not be available until it is completed and accepted by BESAC. This may occur at the February 2003 BESAC meeting. The agenda for the BESAC November 5-6, 2002, BESAC meeting may be found at (http://www.science.doe.gov/production/bes/BESAC/nov02agenda.pdf).

Richard Smith (NSF) discussed the NSF Engineering Directorate Working Group on Energy, which has the objective to “identify (interagency) research opportunities that comprise a broader vision for fundamental energy research.” The group clearly intends to seek both new opportunities and greater interagency coordination. The speaker’s PowerPoint presentation is available subject to the proviso that it is at an early stage and changes are to be expected. Interested parties should contact D. Koelling.

The minutes of the July 16, 2002, meeting were approved. It was moved by R. Gottschall that the slate of officers be elected unanimously. The motion was seconded by C. Sorrell and the motion carried. Accordingly, the officers for 2003 are D. Koelling, chair, and L. Wilson, secretary. Possible dates for the meeting in January, 2003, were discussed. A more or less traditional choice of January 14 appeared to have significant conflicts. Members were asked to advise Koelling and/or Wilson of their availability. The meeting was then adjourned.

Parenthetically, there appeared to be good informal discussion both before and after the meeting.

CALENDAR ITEMS

Oct. 21-25, 2002	Workshop on *Basic Research Needs to Assure a Secure Energy Future*, Gaithersburg, MD, contact Sharon Long
Nov. 5-6, 2002	Basic Energy Sciences Advisory Committee meeting, Gaithersburg, MD, contact Sharon Long
Feb. 25, 2003	Basic Energy Sciences Advisory Committee meeting, Gaithersburg, MD, contact Sharon Long
Feb. 26-28, 2003	DOE Nanoscale Science Centers Workshop, Renaissance Hotel, Washington, D.C. See http://www.ornl.gov/doensrcworkshop/

LIST OF PARTICIPANTS

Altaf Carim	SC-13	Carim@Science.DOE.gov
Yok Chen	SC-13	Yok.Chen@Science.DOE.gov
Robert Gottschall	SC-13	Robert.Gottschall@Science.DOE.gov
Arvind Kini	SC-13	Aravinda.Kini@Science.DOE.gov
Dale Koelling	SC-13	Dale.Koelling@Science.DOE.gov
Harriet Kung	SC-13	Harriet.Kung@Science.DOE.gov
Udaya Rao	FE/NETL	Rao@NETL.DOE.gov
Richard N. Smith	NSF/ENG/CTS	RNSmith@NSF.gov
Charles Sorrell	EE-2F	Charles.Sorrell@EE.DOE.gov
Lane Wilson	FE/NETL	Lane.Wilson@NETL.DOE.gov
Jane Zhu	SC-13	Jane.Zhu@Science.DOE.gov

JANUARY 21, 2003, FORRESTAL BUILDING

EMaCC Chair, Dale Koelling, conducted the meeting; minutes by Lane Wilson, Executive Secretary.

Robert Budnitz, on assignment from LLNL to the Office of Civilian Radioactive Waste Management (RW-40E), gave an overview of the Yucca Mountain radioactive waste (RW) repository. He presented the environmental and safety constraints imposed on the materials systems for RW storage. He stressed that the current design and materials plan can be implemented with a large margin of safety under applicable regulations. The purpose of the science and technology program that is being initiated by RW is to explore opportunities to lower the costs of the facility through possible materials improvements.

All parts in the storage tunnels are non-mechanical. Some of the relevant parts are the “drift shield”, which diverts any moisture that drifts into the tunnel and the “drift invert” which would collect any moisture away from the storage cask and provide a further barrier to ground penetration. The drift invert also performs the structural task of supporting the storage casks. The parts are all made of expensive high grade materials like NiCr superalloys with well-characterized mechanical loading and chemical sorption properties.

Research opportunities may possibly involve surface coatings or non-metallic materials systems. The first casks are scheduled to be loaded into a tunnel at the Yucca Mountain (YM) site in 2010 and the last one in 2034. In order for any new materials to be employed during the later years of the site loading, they will need life cycle validation in the time range of 2010-2020.

There is also a performance confirmation program involving the NRC for the first 100 years of ventilated use before the tunnels are sealed. This could possibly make use of remote sensor R&D.

William Lake (RW-30E) presented the materials needs for the casks used to seal the RW. The casks will be moved by ground transportation to the YM site. The current design was certified by the NRC 40 years ago for adequate safety but like the materials in the YM facility, there are opportunities in materials design to reduce the cost while maintaining performance in areas such as structural containment, radiation shielding, nuclear sub-criticality, and heat dissipation. There are also considerations for weight, impact protection, and personnel barriers.

CALENDAR ITEMS

June 3-5	Materials and Engineering Physics on-site review at Argonne National Laboratory
April 15	Next EMaCC Meeting

APRIL 15, 2003, GERMANTOWN

Dale Koelling, EMaCC Chair, conducted the meeting and minutes were taken by Lane Wilson, Executive Secretary.

Pat Dehmer reported on the BES/BESAC Workshop on "Basic Research Needs to Assure a Secure Energy Future." It was held October 21-25, 2002. The workshop report will function as a "guiding force" in future DOE planning. Thirty seven proposed research directions were put forth. Ten basic research directions were identified and will be explored with subsequent workshops. For example, the direction "Research Towards the Hydrogen Economy" will be examined in a mid-May workshop. Another direction "Materials Research to Transcend Energy Barriers" reflects the fact that about half the proposed research directions had materials issues as technology barriers.

The Workshop Summary emphasized that the problems will require interdisciplinary non-traditional research structures with coordinated integration of the necessary skill sets.

Teresa Fryberger of the Office of Biological and Environmental Research (BER) reported on the work of the Environmental Remediation Sciences group. The research supports the goal of converting waste and contaminants into a more stable form. The major efforts involve the Natural and Accelerated Bioremediation Program (NABIR) and the Environmental Management Science Program (EMSP) with research facilities of the Environmental Molecular Sciences Laboratory (EMSL at PNNL) and the Savannah River Ecology Laboratory (SREL).

A discussion followed contrasting the remediation efforts of BER with issues presented at the last EMaCC meeting by Bob Budnitz concerning radioactive waste management at the Yucca Mountain repository. An EMaCC topical subgroup was suggested and a steering committee of R. Budnitz, T. Fryberger, T. Kiess and R. Gottschall was formed to report back on establishing the sub-group.

The Terms of Reference document (dated 8/24/1993) has been located and will be discussed at the next EMaCC meeting.

A request was made for a web-based archival system of EMaCC reports.

LIST OF PARTICIPANTS

Bob Budnitz	Bob Gottschall	Harriet Kung
Yok Chen	Jim Horwitz	Bill Oosterhuis
Pat Dehmer	Helen Kerch	Mike Soboroff
Sara Dillich	Tom Kiess	Lane Wilson
Teresa Fryberger	Dale Koelling	Jane Zhu

JULY 15, 2003, FORRESTAL BUILDING

Minutes of the July 2003 EMaCC meeting will be published in the FY03 EMaCC Annual Technical 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 (see Appendix). This report summarizes EMaCC activities for FY 2002 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 2002 was Dr. Udaya Rao. The compilation of this report was performed by Dr. Lane Wilson, EMaCC Executive Secretary for FY 2003, 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. Dale Koelling
Office of Science
EMaCC Chair, FY 2003

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
Distributed Energy & Electricity Reliability		
High Temperature Superconductivity	James Daley, EE-2D	202-586-1165
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	202-586-5673
	JoAnn Milliken, EE-2H	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	202-586-1693
	Ray Sutula, EE-2A	202-586-8064

ORGANIZATION	REPRESENTATIVE	PHONE NO.
SCIENCE		
Basic Energy Sciences		
Materials Sciences and Engineering	Pat Dehmer, SC-10	301-903-3081
	Iran L. Thomas, SC-13	301-903-3427
Metals, Ceramics and Engineering	Robert J. Gottschall, SC-13	301-903-3428
	Yok Chen, SC-13	301-903-3428
	Helen Kerch, SC-13	301-903-3428
Condensed Matter Physics and Materials Chemistry	W. Oosterhuis, SC-13	301-903-3426
	Jerry Smith, SC-13	301-903-3426
	Richard Kelly, SC-13	301-903-3426
	Manfred Leiser, SC-13	301-903-3426
	Matesh (Mat) Varma, SC-13	301-903-3209
	Altaf Carim, SC-13	301-903-4895
	Arivinda M. Kini, SC-13	301-903-3565
	Pedro Montano, SC-13	301-903-2347
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		
Technology and International Cooperation	Steve Sherman, NE-20	301-903-2714
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	Jim Carlson, RW-40	202-586-5321
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser, FE-25	301-903-2786

ORGANIZATION OF THE REPORT

The FY 2002 budget summary for DOE Materials Activities is presented on page 8. The distribution of these funds between DOE laboratories, private industry, academia and other organizations is presented in tabular form on page 10.

Following the budget summary is a set of detailed program descriptions for the FY 2002 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 2002 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 2002 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 2002
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$2,989,000
DISTRIBUTED ENERGY & ELECTRICITY RELIABILITY PROGRAM	$32,000,000
High Temperature Superconductivity for Electric Systems	32,000,000
FREEDOMCAR & VEHICLE TECHNOLOGIES PROGRAM	$39,009,000
Materials Technologies Program	39,009,000
Automotive Propulsion Materials	2,845,000
Automotive Lightweight Vehicle Materials	15,750,000
Heavy Vehicle Propulsion System Materials	4,944,000
High Strength Weight Reduction Materials	9,870,000
High Temperature Materials Laboratory	5,600,000
GEOTHERMAL TECHNOLOGIES PROGRAM	$395,000
Geothermal Materials	395,000
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM	$815,000
Fuel Cells Materials Program	815,000
INDUSTRIAL TECHNOLOGIES PROGRAM	$28,167,398
Aluminum Vision Team	10,874,792
Glass Industry of the Future	200,000
Forest and Paper Products	1,950,792
Metal Casting	1,403,000
Industrial Materials for the Future	13,738,814
SOLAR ENERGY TECHNOLOGY PROGRAM	$36,178,000
National Photovoltaics Program	36,178,000
WEATHERIZATION & INTERGOVERNMENTAL PROGRAM	$4,777,020
Financial Assistance Program	4,777,020
Inventions & Innovation (I&I)	2,175,382
National Industrial Competitiveness Through Energy, Environment and Economics (NICE[3])	2,601,638
OFFICE OF SCIENCE	$539,912,655
Office of Basic Energy Sciences	490,258,000
Division of Materials Sciences and Engineering	490,258,000
Office of Advanced Scientific Computer Research	41,254,655
Division of Technology Research	41,254,655
Laboratory Technology Research Program	1,545,000
Small Business Innovation Research Program	37,722,980
Small Business Technology Transfer Research Program	1,986,675
Office of Fusion Energy Sciences	8,400,000
OFFICE OF ENVIRONMENTAL MANAGEMENT	$3,602,996

FY 2002 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES (continued)

	FY 2002
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$12,730,821
Office of Space and Defense Power Systems	3,781,000
Space and National Security Programs	3,781,000
Office of Technology and International Cooperation	8,949,821
Nuclear Energy Plant Optimization	3,555,000
Nuclear Energy Research Initiative	4,569,821
International Nuclear Energy Research Initiative	825,000
NATIONAL NUCLEAR SECURITY ADMINISTRATION	$114,492,000
Office of Naval Reactors	79,200,000[1]
Office of Defense Programs	14,486,000
The Weapons Research, Development and Test Program	14,486,000
Sandia National Laboratories	14,486,000
Los Alamos National Laboratory	15,223,000
Lawrence Livermore National Laboratory	5,583,000
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT	$30,540,000
OFFICE OF FOSSIL ENERGY	$10,343,999
Office of Advanced Research	10,343,999
Fossil Energy Advanced Research Materials Program	6,745,999
Advanced Metallurgical Processes Program	3,598,000
TOTAL	**$855,952,889**

[1]This excludes $51.7 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	$1,880,000	$1,034,000	$75,000	$0	$2,989,000
Distributed Energy & Electricity Reliability Program	$12,128,000	$16,545,000	$3,000,000	$327,000	$32,000,000
FreedomCAR & Vehicle Technologies	$24,413,000	$11,161,000	$2,145,000	$1,290,000	$39,009,000
Geothermal Technologies Program	$395,000	$0	$0	$0	$395,000
Hydrogen, Fuel Cells & Infrastructure Technologies Program	$600,000	$0	$215,000	$0	$815,000
Industrial Technologies Program	$13,358,792	$10,105,792	$4,430,814	$272,000	$28,167,398
Solar Energy Technology Program	$36,178,000	$0	$0	$0	$36,178,000
Weatherization & Intergovernmental Program	$0	$4,537,142	$239,878	$0	$4,777,020
Office of Science	$431,470,000	$39,709,655	$67,710,000	$1,023,000	$539,912,655
Office of Environmental Management	$2,225,996	$0	$1,377,000	$0	$3,602,996
Office of Nuclear Energy, Science and Technology	$10,193,398	$1,510,000	$827,423	$200,000	$12,730,821
National Nuclear Security Administration	$114,492,000	$0	$0	$0	$114,492,000
Office of Civilian Radioactive Waste Management	$30,540,000	$0	$0	$0	$30,540,000
Office of Fossil Energy	$8,943,000	$200,999	$780,000	$420,000	$10,343,999
TOTALS	**$686,817,186**	**$84,803,588**	**$80,800,115**	**$3,532,000**	**$855,952,889**

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 2002
OFFICE OF BUILDING TECHNOLOGIES - GRAND TOTAL	$2,989,000
OFFICE OF BUILDING RESEARCH AND STANDARDS	$2,989,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	1,305,000
Non-HCFC Closed-Cell Foam Insulation	150,000
Hygrothermal Material Property Measurements & Modeling Upgrades and Applications	855,000
Insulation Materials Performance & Application	150,000
Sub-Ambient Pipe Insulation Materials and Systems	75,000
Floor Tile with Phase Change Materials	75,000
FENESTRATION MATERIALS DEVELOPMENT	$1,684,000
Development of Electrochromic Materials and Coatings	1,486,000
Development of Aerogel Materials for R10/ inch Transparent Window Insulation	198,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

OFFICE OF BUILDING RESEARCH AND STANDARDS

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.

The program objectives are:

1) The 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**
$150,000
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**
$855,000
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 America 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. **CONVENTIONAL MATERIALS PERFORMANCE**
   $150,000
   DOE Contact: Marc LaFrance (202) 586-9142
   ORNL Contact: Ken Wilkes (865) 574-5931

This project is for the development of accurate and reproducible data for use by the building materials community, improved test procedures to determine the thermal properties of existing, as well as advanced, insulations, interacting with the building materials research community, manufacturers, trade associations, professional societies, compliance groups and local government, and making and disseminating recommendations on appropriate usage of thermal insulation to conserve energy.

Keywords: Insulation, Buildings

4. **SUB-AMBIENT PIPE INSULATION MATERIALS AND SYSTEMS**
   $75,000
   DOE Contact: Marc LaFrance (202) 586-9142
   ORNL Contact: Bill Miller (865) 574-2013

Pipe thermal insulations are rated by the thermal resistance as measured in pipe testing apparatus in conformance with ASTM C335. The scope of ASTM C335 limits its use to piping systems operating at temperatures above ambient. Numerous ASTM material specifications specify the use of these materials on pipes operating below ambient conditions. There are no test methods or test facilities available for undertaking these measurements.

Pipe insulations applied to piping operating at sub-ambient conditions are also a major concern within ASHRAE. These insulation systems can have severe moisture-related problems due to the unidirectional nature of their vapor drive. Attempts to address the rash of failures to these systems due to moisture ingress leading to loss in energy efficiency as well as mechanical failure are planned.

Keywords: Piping, Moisture, Insulation, Properties

5. **PHASE CHANGE MATERIALS IN FLOOR TILES FOR THERMAL STORAGE**
   DOE $75,000, Colorado State Univ. cost-sharing $18,000
   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

6. **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 $836,000, Sage cost-sharing $235,000
SAGE Electrochromic Inc. Contact: 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.

$500,000
LBNL Contact: 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 Contact: 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 ultraviolet 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

7. **DEVELOPMENT OF TRANSPARENT AEROGELS R10/INCH FOR WINDOWS**
   DOE $198,000, Aspen Aerogels cost-sharing $50,000
   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

DISTRIBUTED ENERGY & ELECTRICITY RELIABILITY PROGRAM

	FY 2002
DISTRIBUTED ENERGY & ELECTRICITY RELIABILITY PROGRAM - GRAND TOTAL	$32,000,000
HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS	$32,000,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$32,000,000
The 2nd Generation Wire Initiative	10,100,000
Partnership with Industry	8,000,000
Strategic Research	13,900,000

DISTRIBUTED ENERGY & ELECTRICITY RELIABILITY PROGRAM

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). Longer-term wire research activities are investigating TBCCO (thallium barium calcium copper oxide) and other compounds for coated conductors, as well as the investigation of 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 benefit 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 2002 saw a reorganization of the Superconductivity Program’s parent organization, the Office of Energy Efficiency and Renewable Energy (EERE). The High Temperature Superconductivity group became an element of the Distributed Energy and Electricity Reliability (DEER) Program. The DEER Program aims to improve the efficiency and reliability of the nation’s electricity transmission system.

FY 2002 also saw a decline in the annual operating budget of High Temperature Superconductivity for Electric Systems of approximately 16 percent from the prior year. This decline represented the first reduction in the program’s budget in the last eight years. The result was somewhat lower spending on capital equipment for national laboratories, as well as the postponement of the awarding of several new industry-led demonstration projects. Results that will be presented at the Peer Review in summer 2003 will determine what, if any, effect the reduction will have in achieving milestones for the long term commercialization of the technology. The DOE contact is Jim Daley, 202-586-1165.

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

8. **THE 2ND GENERATION WIRE INITIATIVE**
$10,100,000
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
Sandia National Laboratory Contact: Paul Clem
(505) 845-7544
Industry Partners: American Superconductor
Contact: John Scudiere (508) 836-4200
Intermagnetics General Corp. Contact:
Phillip Pellegrino (518) 346-1414
Oxford Superconducting Technology Contact:
Seung Hong (732) 541-1300
3M Contact: Jonathan Storer (651) 733-6462
MicroCoating Technologies Contact: Shara Shoup
(678) 287-2478

The 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 2002 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.

IBAD Research - Program partners were completing the first phase of research on the IBAD approach. Electron beam evaporation is 3M's selected method of deposition of all the layers. ORNL worked to characterize bare, textured nickel and films grown by a variety of techniques, and to develop buffer layer and superconductor deposition technology. ORNL continued pursuing a promising alternative to in-situ formation of the YBCO film, by electron beam co-evaporation of Y, Ba, and Cu. ORNL scientists worked on determining the thickness limits of epitaxial film formation, and assessing the feasibility of rapid precursor depositions for the ex-situ precursor reaction process.

YBCO/RABiTS - Development and demonstration of the fabrication of lengths of YBCO/RABiTS using MOCVD technology continued. Mechanical and processing conditions needed to develop the desired surface texture and smoothness of the bare nickel were investigated. 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

9. **PARTNERSHIP WITH INDUSTRY**
$8,000,000

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 2002, 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 2002 or early 2003.

Project subtasks are as follows:

Current Controllers - LANL Researchers continued efforts to optimize the performance of a demonstration HTS Current Controller developed by General Atomics. Current controllers 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 controllers offer better protection and improved system flexibility, reliability, and performance. Los Alamos National Laboratory (LANL) scientists completed the optimization of one of the devices three large coils, and work is beginning on the other two.

LANL Contact: Dean Peterson (505) 665-3030

Motors - The project, led by Rockwell Automation, completed operational testing of a 1,000 horsepower (hp) motor in 2001. In 2002 design studies for a 5,000 horsepower motor using HTS tape for the windings were underway. 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

Cold Dielectric Superconducting Transmission Cable - Southwire Company 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. Southwire began work, in conjunction with Oak Ridge National Laboratory, on a new design for a 100-meter, three phase power cable to be installed at a substation in Columbus, Ohio. The project builds on an earlier SPI success, the 30-meter, three-phase HTS cable that was completed in 2000 and feeds electricity to three Southwire manufacturing facilities.

Southwire Contact: David Lindsay (770) 832-4916

Warm Dielectric Superconducting Transmission Cable - A team led by Pirelli Cables and Systems and including Detroit Edison, American Superconductor, and Los Alamos National Lab continued efforts to operate a prototype HTS cable in a utility substation in Detroit. The project has had to overcome problems with vacuum leaks in the cable, and Pirelli hopes to commission one phase of the cable in the next few months. 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 2002 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 late in 2002 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 2002, the team completed the assembly of the transformer and began testing of the unit. Some high-voltage problems have surfaced, and Waukesha and ORNL are working to overcome these obstacles.

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 began conceptual designs and component acquisition/fabrication.

ORNL Contact: Bob Hawsey (865) 574-8057

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

10. **STRATEGIC RESEARCH**
$13,900,000
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 2002. 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.

ORNL funded two university research and development projects in FY 2002. Researchers at Stanford University investigated ion-beam assisted deposition of buffer layers and in-situ deposition of YBCO by electron beam evaporation. The University of Wisconsin conducted research on BSCCO critical currents and microstructures, YBCO coated conductor microstructure, and pulse tube cryocooler technology.

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, Thallium Conductor, Bismuth Conductor

FREEDOMCAR & VEHICLE TECHNOLOGIES

	FY 2002
FREEDOMCAR & VEHICLE TECHNOLOGIES - GRAND TOTAL	$39,009,000
MATERIALS TECHNOLOGIES PROGRAM	$39,009,000
AUTOMOTIVE PROPULSION MATERIALS	$2,845,000
Technical Project Management	300,000
Low-Cost, High Energy Product Permanent Magnets	250,000
Characterization of Permanent Magnets	50,000
Carbon Foam Thermal Management Materials for Electronic Packaging	200,000
Mechanical Reliability of Electronic Ceramics and Electronic Ceramic Devices	150,000
Microwave-regenerated Diesel Engine Exhaust Particulate Filter Technology	450,000
Rapid Surface Modifications of Aluminum Engine Block Bores for Weight Reduction	200,000
Material Support for Nonthermal Plasma Diesel Engine Exhaust Emission Control	200,000
Low-Friction Coatings for Fuel Cell Air Compressors	200,000
Microstructural Characterization of PEM Fuel Cells	200,000
Inorganic Polymer Electrolyte Membrane Electrode/support Development	75,000
Carbon Foam for Radiators for Fuel Cells	125,000
Fabrication of Small Injector Orifices	180,000
Technology for Producing Small Holes in Advanced Materials	115,000
Electrochemical NO_x Sensor for Monitoring Diesel Emissions	150,000
AUTOMOTIVE LIGHTWEIGHT VEHICLE MATERIALS	$15,750,000
Low-Cost High Performance Wrought Aluminum Components for Automotive Applications	450,000
Low-Cost High Performance Cast Light Metals for Automotive Applications	500,000
Advanced Materials and Processes for Automotive Applications	550,000
Technology Assessment and Evaluation	1,650,000
Advanced Joining Technologies	1,500,000
High Strain Rate Deformation of Materials	925,000
Reinforced Composite Materials, Durability, and Enabling Technologies	750,000
USAMP Cooperative Agreement	6,300,000
Development of Low-Cost Carbon Fiber	1,900,000
Recycling	350,000
Structural Reliability of Lightweight Glazing Alternatives	350,000
High Rate Processing Technologies for Polymer Composite Materials	525,000
HEAVY VEHICLE PROPULSION MATERIALS	$4,944,000
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
Diesel Engine Particulate Filter	300,000
Development of NO_x Sensors for Heavy Vehicle Applications	200,000
Field Emission Analytical Microscopy for Characterization of Catalyst Microstructures and Deactivation Mechanisms	200,000
Advanced Materials for Lightweight Valve Train Components	189,000
Thick Thermal Barrier Coatings (TTBCs) for Low Emission, High Efficiency Diesel Engine Components	200,000

FREEDOMCAR & VEHICLE TECHNOLOGIES (continued)

	FY 2002
HEAVY VEHICLE PROPULSION MATERIALS (continued)	
Mechanical Characterization	85,000
NDE of Diesel Engine Components	200,000
Durability of Diesel Engine Component Materials	200,000
Life Prediction of Diesel Engine Components	200,000
Low-Cost Manufacturing of Precision Diesel Engine Components	235,000
Cylindrical Wire EDM and Temperature Measurement	75,000
Development of Low-Cost Austenitic Stainless Diesel Engine Components with Enhanced High-Temperature Reliability	160,000
TiAl Nanolaminate Composites	100,000
Synthesis of Powders for Titanium Carbide/Nickel Aluminide Cermets	75,000
Diesel Exhaust Gas Recirculation Corrosion Effects	50,000
Durability of Diesel Engine Component Materials	200,000
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	100,000
HIGH STRENGTH WEIGHT REDUCTION MATERIALS	$9,870,000
Design, Analysis and Development of Lightweight Frames for Truck and Bus Applications	1,275,000
Development of Advanced Casting Technologies for Production of High Integrity Truck Components	800,000
Advanced Forming Technologies for Lightweight Alloys	675,000
Development of Carbon Monoliths for Safe, Low Pressure Adsorption Storage and Release Natural Gas	600,000
Improved Materials for Heavy Vehicle Brake and Friction Applications	675,000
High Conductivity Carbon Foams for Thermal Management	125,000
Advanced Joining Technology Development	500,000
Development of Advanced Materials for Heavy Vehicle Applications	1,250,000
Implementation of Lightweight Materials in Heavy Vehicle Structural Applications	2,470,000
Technology Assessment and Evaluation	1,500,000
HIGH TEMPERATURE MATERIALS LABORATORY	$5,600,000
The High Temperature Materials Laboratory User Program	5,600,000

FREEDOMCAR & VEHICLE TECHNOLOGIES

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 Technologies R&D is conducted by the Materials Team to address critical needs of automobiles and heavy vehicles. These activities are closely coordinated with other Department programs and those of other Federal and non-governmental organizations to ensure non-duplication of efforts. 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. Much of the research that is focused on automobiles is conducted in cooperation with the auto industry through the United States Consortium for Automotive Research (USCAR) through the FreedomCAR partnership. Likewise, the 21st Century Truck Partnership is the umbrella organization which coordinates much of the heavy vehicle materials research with the trucking industry.

Within the FreedomCAR program, 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 Technologies program. The Materials Technologies program addresses: a) *Automotive Propulsion Materials* to develop material solutions for electric drive systems and engine and emission control systems, and b) *Automotive Lightweight Vehicle Materials* to reduce vehicle weight and thereby reduce fuel consumption. The program seeks to develop advanced composites and metals 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. The DOE contacts are Rogelio Sullivan (202) 586-8042, for automotive propulsion materials and Joseph Carpenter, 202-586-1022, for automotive lightweight vehicle materials.

Within the Materials Technologies program, the truck, bus, and heavy vehicle materials research are addressed through a) *Heavy Vehicle Propulsion System Materials,* and b) *High Strength Weight Reduction 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 turbochargers and superchargers; 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. In the area of high strength weight reduction materials, energy savings from commercial trucking is possible through application of 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 contact is Sid Diamond (202) 586-8032.

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

11. **TECHNICAL PROJECT MANAGEMENT**
$300,000
DOE Contact: N. L. Garland (202) 586-5673
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

12. **LOW-COST, HIGH ENERGY PRODUCT PERMANENT MAGNETS**
$250,000
DOE Contact: N. L. Garland (202) 586-5673
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. The solenoid better aligns the magnetic domains of NdFeB powder during pressing into green compacts. The energy product (MGOe) and remnant field Br(kG) of magnets produced in this facility showed a strong dependence on the magnitude of the alignment field H(T). Achieved energy product improvements of 15% for thin near-final-shape magnets, production of which is the current cost-saving thrust in the PM industry. Additional PMs made with relatively small length-to-diameter ratio (L/D<0.5) supports the previous findings. Carried out electromagnetic code study of grain alignment in powder compacts. The results show that the distortion of the alignment field (caused by the self-field of the compact) is proportional to the density of the compact and inversely proportional to the magnitude of the alignment field. These results will help to provide scale up design rules to industry. Collaborated with Oak Ridge National Laboratory and Ames Laboratory on characterizing the microscopic texture (alignment) of PMs made at Argonne and on processing the NdFeB powder for bonded PMs at the 9-Tesla superconducting magnet at ANL; respectively.

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

13. **CHARACTERIZATION OF PERMANENT MAGNETS**
$50,000
DOE Contact: N. L. Garland (202) 586-5673
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

14. **CARBON FOAM THERMAL MANAGEMENT MATERIALS FOR ELECTRONIC PACKAGING**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
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. Research with the National Security Agency has shown that the carbon foams can be used as an evaporative substrate in a totally passive heat pipe and allow up to 115 W/cm^2 power density in the electronics and still maintain the required low temperatures of operation of 56˚C. In addition, improvements in the fabrication process resulted in foams with a more uniform density distribution, higher compressive strengths (up to 100% higher) and, hence, increased durability and machinability.

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

15. **MECHANICAL RELIABILITY OF ELECTRONIC CERAMICS AND ELECTRONIC CERAMIC DEVICES**
$150,000
DOE Contact: N. L. Garland (202) 586-5673
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.

Received three series of polymer film samples from SNL and characterized them using a mechanical properties microprobe. Performed indentation studies with a mechanical properties microprobe to characterize hardness and Young's modulus on a suite of SNL dielectric films. Purchased a universal test frame with film-gripping capabilities and that can perform tensile test at high temperatures, and verified its operation and accuracy.

Keywords: Electronics, Failure Analysis, Life Prediction, Mechanical Properties, Multilayer Capacitors

16. **MICROWAVE-REGENERATED DIESEL ENGINE EXHAUST PARTICULATE FILTER TECHNOLOGY**
$450,000
DOE Contact: N. L. Garland (202) 586-5673
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. During the year a microwave regeneration system was designed and built that is capable of performing on a PNGV-type diesel engine. The microwave filter system demonstrated 95 percent efficiency on a 1.9-L Volkswagen engine in a test cell at Oak Ridge National Laboratory and 95% filter regeneration frequency on a Volkswagen Jetta vehicle. An improved pleated-filter cartridge microwave filter system was designed and bench tested for installation and track testing on a Ford F-250 7.3-L diesel pickup. The microwave filter system fuel penalty, as calculated from these test results, was an impressively low 0.3 percent and the engine exhaust backpressure was reduced significantly with the pleated filter cartridge.

Keywords: Carbon Particulates, Diesel, Filters, Microwave Regeneration

17. **RAPID SURFACE MODIFICATIONS OF ALUMINUM ENGINE BLOCK BORES FOR WEIGHT REDUCTION**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: C. Blue (865) 574-5112

Innovative, rapid, high-density surface modification processes are being used to develop a new, durability-enhancing coating for automotive applications such as aluminum engine block cylinder bores, compressor housings, fuel pumps and sealing surfaces. The concern about one such coating (Fe-Cr-B-Mn-Si) was associated with the porosity and hardness of the coating and the bonding characteristics of the coating to the substrate. Experiments were conducted by varying the arc lamp's reflector geometry, amperage (i.e., power density), and pulse or exposure time. It was shown that there was a significant reduction in porosity, increased coating hardness, and adequate metallurgical bonding. This research demonstrates the plasma arc lamp's capability to rapidly fuse coatings in an air environment. A procedure was also developed using the tungsten halogen lamp to dramatically reduce the time required to cure an epoxy used to join automotive body panels. The process was so successful, that is was implemented on a production line for the Ford Lincoln LS vehicle.

Keywords: Aluminum, Cost Reduction, Engines, Hard Coatings, Wear

18. **MATERIAL SUPPORT FOR NONTHERMAL PLASMA DIESEL ENGINE EXHAUST EMISSION CONTROL**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
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. Ceramic dielectric components that were produced using the new fabrication process which utilizes commercially available tape cast ceramic materials were tested at PNNL. Three of the ceramic components were stacked in a test fixture and connected to a voltage supply to generate a plasma discharge. The tests demonstrated that the components produce a uniform plasma with no dielectric breakdown under operating conditions. In a companion effort, a sealing glass was identified for joining together the ceramic components of the NTP reactor assembly. The sealing glass will be used to bond together the stack of dielectric plates and to seal the assembly to prevent the escape of exhaust gases.

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

19. **LOW-FRICTION COATINGS FOR FUEL CELL AIR COMPRESSORS**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ANL Contact: G. R. Fenske (630) 252-5190

The objective of this work is to develop and evaluate the friction and wear performance of low-friction materials and coatings for fuel cell air compressor/expander systems. The impact of Argonne's near frictionless carbon (NFC) coating on the performance of a novel journal air bearing (developed by Meruit) was evaluated in a series of bearing tests. The NFC coating enabled the development of the low-cost bearing technology and was successfully demonstrated in a test that experienced over 10,000 start-stop cycles (without the coating, the bearing seized during the first cycle). Argonne also worked closely with Mechanology, LLC to evaluate the friction and wear properties of materials for a novel air compressor they were developing for DOE. The study, which is still in progress, has identified the importance of thermal conductivity as a key property in determining the tribological performance of polymers at elevated speeds.

Keywords: Air Compressors, Carbon, Friction, Near Frictionless Coating, Scuffing, Wear

20. **MICROSTRUCTURAL CHARACTERIZATION OF PEM FUEL CELLS**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: D. Blom
(865) 241-3898

The objectives of this effort are to optimize the catalyst microstructure and distribution in membrane electrode assemblies (MEAs) for low cost and high performance and to understand the effects of microstructure and microchemical composition on the performance and aging characteristics of the fuel cell. A new cryo-ultramicrotomy facility was inaugurated at the High Temperature Materials Laboratory at Oak Ridge National Laboratory. Cryo-ultramicrotomy is believed to be a key preparation step for thinner MEA cross-sections that will allow higher-resolution and more definitive characterization. An MEA aged to failure at 1200 hours of operation (using a very aggressive aging schedule) was characterized for its chemical homogeneity and catalyst particle size. Unlike previous aged MEAs, no evidence of a chemically distinct layer at the membrane/electrode interface was seen. We believe the aging protocol used was so aggressive that massive bulk membrane failure occurred before the chemical aging of the membrane interface. Both the cathode and anode catalyst particles coarsened during the aging process, though the particles in the anode grew a statistically significant amount more than the cathode catalyst particles. Careful development of relevant accelerated aging protocols is clearly necessary to provide data applicable to actual in-user conditions.

Keywords: Catalysts, Fuel Cells, Platinum Membrane Electrode Assemblies, TEM Characterization

21. **INORGANIC POLYMER ELECTROLYTE MEMBRANE ELECTRODE/SUPPORT DEVELOPMENT**
$75,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: M. A. Janney
(865) 574-4281

The goal of this effort is to develop electrically conducting electrodes/supports and catalytically active ceramic sandwich layers for use in inorganic microporous PEM membranes based on nanoparticles of TiO_2 and Al_2O_3. The materials developed in this project will be used as substrates at the University of Wisconsin for the fabrication of microporous inorganic proton exchange membranes. A process was developed to fabricate electrically conducting, porous nickel materials that will be initially used as substrates. An improved graphite fiber-based substrate/electrode having the requisite chemical compatibility with the PEM environment is being developed to replace the porous nickel. After successful development of the substrates, a second process was devised to deposit microporous titania with carefully controlled particle size and permeability onto the substrate. Sandwich layers of microporous titania on porous nickel were fabricated and shipped to the University of Wisconsin. The nickel/titania sandwich material was found to be an appropriate surface upon which to deposit the nanoparticle membrane.

Keywords: Ceramics, Fuel Cells, Membranes, Titanium Oxide

22. **CARBON FOAM FOR RADIATORS FOR FUEL CELLS**
$125,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: A. D. McMillan
(865) 241-4554

The purpose of this work is to develop compact, lightweight, and more efficient radiators for fuel-cell-powered vehicles utilizing Oak Ridge National Laboratory’s unique, high-conductivity carbon foam. Research focused on durability and environmental characterization in this year. Results have shown that vibration has no apparent effect on the foams material properties or the soldered interface. However, it was shown that a significant decrease in thermal properties (up to 50%) can be found under corrosion with radiator fluid and certain solders and base plates. It was found that the corrosion is attacking the substrate and not the foam, and therefore, methods to protect the substrate will prove useful in decreasing corrosion problems. Last, corrugated heat exchangers were found to reduce the pressure drop by more than an order of magnitude, while affecting the heat transfer minimally.

Keywords: Carbon Foam, Heat Exchangers, Heat Transfer, Radiators

23. **FABRICATION OF SMALL INJECTOR ORIFICES**
$180,000
DOE Contact: N. L. Garland (202) 586-5673
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 125 mm in diameter. Ideally, however, the orifice diameter should be reduced to 50 mm 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. Aqueous-based and vacuum-based processes are being considered, with an initial focus on electroless coating processes. During the first year of this project, an electroless plating process was selected and developed to coat the inner surfaces of commercial fuel injectors. The process was demonstrated on commercial injectors as being able to reduce the orifices from 0.2 mm to 0.1 mm. Work is in progress to achieve a 0.05 mm diameter orifice.

Keywords: Fuel Injectors, Nozzles, Orifice, Coating

24. **TECHNOLOGY FOR PRODUCING SMALL HOLES IN ADVANCED MATERIALS**
$115,000
DOE Contact: N. L. Garland (202) 586-5673
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. Two related approaches were developed for producing holes in gelcast alumina ceramic. The basic approach for forming the holes was to incorporate either organic fibers or metal wires within the molded gelcast ceramic green (unsintered) body. The organic fibers burn away during the high-temperature sintering process that is used to densify the ceramic and leave fine holes in the dense material. The metal wires can be removed from the green ceramic prior to sintering, leaving holes that remain after densification. Using these methods, holes that were about 30µm in diameter and as long as 20mm were produced.

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

25. **ELECTROCHEMICAL NO_x SENSOR FOR MONITORING DIESEL EMISSIONS**
$150,000
DOE Contact: N. L. Garland (202) 586-5673
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 NO sensor. The sensor operates at 650ºC, and has excellent NO sensitivity and a fast response time of less than 1 second. The high signal-to-noise ratio indicates a short-term sensitivity limit £ 25 ppm NO. Current efforts are focused on the long-term stabilization of the electrode microstructure, which tends to coarsen during amperometric operation. Coarsening of the electrode microstructure can lead to drifting of the sensor baseline. Future efforts will be directed towards continued refinement of the electrode material/microstructure, investigation of the cross sensitivity to other gasses, and sensor integration.

Keywords: NO_x, Electrochemical Sensor, CIDI, Diesel Exhaust

AUTOMOTIVE LIGHTWEIGHT VEHICLE MATERIALS

26. **LOW-COST HIGH PERFORMANCE WROUGHT ALUMINUM COMPONENTS FOR AUTOMOTIVE APPLICATIONS**
$450,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: LANL, PNNL
Industry Partners: Alcoa

The objectives of this effort are: to develop electromagnetic forming (EMF) technology that will enable the economic manufacture of automotive components from aluminum sheet; and to evaluate structural extrusion formability, to experimentally validate stress-based forming limits, and to validate enhanced formability through the application of non-proportional loading.

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

27. **LOW-COST HIGH PERFORMANCE CAST LIGHT METALS FOR AUTOMOTIVE APPLICATIONS**
$500,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: LLNL, ORNL, SNL, INEEL, ANL
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

28. **ADVANCED MATERIALS AND PROCESSES FOR AUTOMOTIVE APPLICATIONS**
$550,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: PNNL
Industry Partners: USAMP (Ford, GM, Chrysler), MC-21

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.

Keywords: Metal Matrix Composites, Aluminum, Casting, Brake Rotors

29. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,650,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
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

30. **ADVANCED JOINING TECHNOLOGIES**
$1,500,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
Laboratory Partners: LBNL, ORNL, PNNL

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

31. **HIGH STRAIN RATE DEFORMATION OF MATERIALS**
$925,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: AISI

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 the 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

32. **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

33. **USAMP COOPERATIVE AGREEMENT**
$6,300,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORO Contact: Mary Rawlins (865) 576-0823
University Partners: University of Tulsa, University of Michigan, 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

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, Development of Manufacturing Methods of Fiber Preforms, 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

34. **DEVELOPMENT OF LOW-COST CARBON FIBER**
$1,900,000
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.

35. **RECYCLING**
$350,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Phil Sklad (865) 574-5069
ANL Contact: George Fenske (630) 252-5190
Laboratory Partners: ANL
Industry Partners: Vehicle Recycling Partnership

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

36. **STRUCTURAL RELIABILITY OF LIGHTWEIGHT GLAZING ALTERNATIVES**
$350,000
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

37. **HIGH RATE PROCESSING TECHNOLOGIES FOR POLYMER COMPOSITE MATERIALS**
$525,000
DOE Contact: Joseph Carpenter (202) 586-1022
ORNL Contact: Dave Warren (865) 574-9693
PNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: ORNL, PNL
Industry Partners: USCAR (DaimlerChrysler, Ford, General Motors), Delphi

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.

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

HEAVY VEHICLE PROPULSION MATERIALS

38. **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

39. **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 2002 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 2003 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

40. **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

41. **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

42. **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

43. **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 will cover the following technologies. 1. Lean-NOx Catalysis:
Because of the inherently low hydrocarbon concentration in diesel exhaust, any NOx 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 NOx including Lean-NOx and Plasma Assisted Catalysis technologies. 2. NOx Sensor: In most aftertreatment strategies, multiple NOx sensors will be required to monitor exhaust NOx 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 NOx in the diesel exhaust environment.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

44. **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 FY02 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

45. **DIESEL ENGINE PARTICULATE FILTER**
$300,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
Cummins Contact: Randy Stafford (812) 377-3279

The objective of this effort is the development of a diesel engine exhaust particulate filter that will allow the 2007 EPA emission requirements to be met while maintaining, or improving, the durability and fuel efficiency of the engine.

Keywords: Diesel Engine, Exhaust Emissions, Particulate Emissions

46. **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

47. **FIELD EMISSION ANALYTICAL 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 NO_x-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

48. **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

49. **THICK THERMAL BARRIER COATINGS (TTBCs) FOR LOW EMISSION, HIGH EFFICIENCY 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

50. **MECHANICAL CHARACTERIZATION**
$85,000
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

51. **NDE OF DIESEL ENGINE COMPONENTS**
$200,000
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

52. **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 2001, 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 2002, 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

53. **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

54. **LOW-COST MANUFACTURING OF PRECISION DIESEL ENGINE COMPONENTS**
$235,000
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

55. **CYLINDRICAL WIRE EDM AND TEMPERATURE MEASUREMENT**
$75,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
N. C. State 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

56. **DEVELOPMENT OF LOW-COST AUSTENITIC STAINLESS DIESEL ENGINE COMPONENTS WITH ENHANCED HIGH-TEMPERATURE RELIABILITY**
$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

57. **TiAl NANOLAMINATE COMPOSITES**
$100,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
LLNL Contact: Luke Hsuing

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

58. **SYNTHESIS OF POWDERS FOR TITANIUM CARBIDE/NICKEL ALUMINIDE CERMETS**
$75,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
U. 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

59. **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

60. **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 support the 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. Emphasis is placed on parts that are subjected to high contact pressures and/or operating temperatures, like fuel injector plungers and emissions control system components where scuffing is a concern.

Keywords: Friction, Scuffing, Fuel Injectors

61. **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

62. **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

63. **TESTING STANDARDS**
$100,000
DOE Contact: Sidney Diamond (202) 586-8032
ORNL Contact: D. R. Johnson (865) 576-6832
NIST Contact: George Quinn (303) 492-3759

In FY 2002, work will focus on the following American Society of Testing and Materials and International Organization for Standards standards:

- Revisions will be completed on three ASTM standards: Flexural Strength Standard C 1161, Fracture Toughness Standard C 1421 and Fractographic Analysis Standard C 1322.
- The Surface Crack in Flexure (SCF) test method will be completed as an ISO standard test.
- A first ballot draft of the new flexural strength standards for cylindrical rods will be completed.

Keywords: Standards, ASTM, Fracture Toughness, Flexural Strength

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

64. **DESIGN, ANALYSIS AND DEVELOPMENT OF LIGHTWEIGHT FRAMES FOR TRUCK AND BUS APPLICATIONS**
$1,275,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Autokinetics, DaimlerChrysler, Alcoa, Tower Automotive, Auto/Steel Partnership

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, MMCs and polymer matrix composites.

Keywords: Frames, Manufacturing, Lightweight, Trucks, Buses

65. **DEVELOPMENT OF ADVANCED CASTING TECHNOLOGIES FOR PRODUCTION OF HIGH INTEGRITY TRUCK COMPONENTS**
$800,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
PNNL Contact: Mark Smith (509) 376-2847
Laboratory Partners: ORNL, PNNL, Albany Research Labs
Industry Partners: Freightliner, PACCAR, Alcoa

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

66. **ADVANCED FORMING TECHNOLOGIES FOR LIGHTWEIGHT ALLOYS**
$675,000
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, Magnesium, Aluminum

67. **DEVELOPMENT OF CARBON MONLITHS FOR SAFE, LOW PRESSURE ADSORPTION STORAGE AND RELEASE NATURAL GAS**
$600,000
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

68. **IMPROVED MATERIALS FOR HEAVY VEHICLE BRAKE AND FRICTION APPLICATIONS**
$675,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL
Industry Partners: Honeywell

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

69. **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

70. **ADVANCED JOINING TECHNOLOGY DEVELOPMENT**
$500,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
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, Joining

71. **DEVELOPMENT OF ADVANCED MATERIALS FOR HEAVY VEHICLE APPLICATIONS**
$1,250,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ANL, NIST, ORNL, PNNL

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

72. **IMPLEMENTATION OF LIGHTWEIGHT MATERIALS IN HEAVY VEHICLE STRUCTURAL APPLICATIONS**
$2,470,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contacts: Phil Sklad (865) 574-5069 and Dave Warren (865) 574-9693
PNNL Contact: Mark Smith (509) 376- 2874
Laboratory Partners: ORNL, PNNL
Industry Partners: Freightliner, PACCAR, Delphi, Volvo

The objective of this project is to develop cost-effective manufacturing processes and design procedures for 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 is the goal of each research effort.

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

73. **TECHNOLOGY ASSESSMENT AND EVALUATION**
$1,500,000
DOE Contact: Sid Diamond (202) 586-8032
ORNL Contact: Phil Sklad (865) 574-5069
Laboratory Partners: ORNL

The objective of these activities is: to 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

74. **HIGH TEMPERATURE MATERIALS LABORATORY USER PROGRAM**
$5,600,000
DOE Contact: Sidney Diamond (202) 586-8032
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 2002
GEOTHERMAL TECHNOLOGIES PROGRAM - GRAND TOTAL	$395,000
GEOTHERMAL MATERIALS	$395,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$395,000
Non-Destructive Testing of Corrosion- and Erosion-Induced Damage in Geothermal Piping Systems	235,000
Structural Response Analysis for Well Cements	160,000

GEOTHERMAL TECHNOLOGIES PROGRAM

GEOTHERMAL MATERIALS

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.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

75. **NON-DESTRUCTIVE TESTING OF CORROSION- AND EROSION-INDUCED DAMAGE IN GEOTHERMAL PIPING SYSTEMS**
$235,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M.L. Berndt (631) 344-3060 and A. J. Philippacopoulos (631) 344-6090

This project addresses the need for improved instrumentation and non-destructive testing (NDT) to detect corrosion and erosion-corrosion of geothermal piping systems. Emphasis is placed on evaluating the suitability of long-range NDT methods for on-line inspection. The research involves: (a) theoretical investigation of NDT methods as applied to specific problems encountered in geothermal facilities; (b) field demonstration and evaluation of NDT methods with emphasis on on-line, long range techniques; and (c) integration of the results from NDT with remaining strength and life assessment. Ultrasonic guided wave methods have been identified as having the greatest potential. Currently available guided wave systems for testing piping use either a ring arrangement of multiple dry coupled piezoelectric transducers clamped to the external pipe surface or a magnetostrictive sensor strip wrapped around the pipe. Piezoelectric transducers in current use have a temperature limitation of approximately 140°C (284°F) and, consequently, their application to in geothermal piping is restricted to relatively low temperature conditions (i.e., injection piping or during plant shutdown). The magnetostrictive system has greater range of application owing to its ability to withstand higher temperatures. In order to facilitate field implementation, limited modeling studies were carried out. The latter involved numerical evaluation of necessary dispersion relations for the propagation of elastic waves in waveguides. Field demonstration of the magnetostrictive system is planned. The field tests will establish the advantages, limitations and economic benefit of implementing guided wave NDT in geothermal plants. Of specific interest is the inspection range for pipes with different complexity as well as the impact of degree of scaling and presence of cement liners.

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

76. **STRUCTURAL RESPONSE ANALYSIS FOR WELL CEMENTS**
$160,000
DOE Contact: R. LaSala (202) 586-4198
BNL Contacts: M.L. Berndt (631) 344-3060 and A. J. Philippacopoulos (631) 344-6090

This project investigates the mechanical behavior of geothermal well cements. It employs detailed experimental testing confirmed by numerical modeling of the structural response due to pressure and temperature conditions. It is demonstrated that adequate materials characterization and selection of cements used for the completion of all types of wells (i.e., geothermal, oil and gas) must be based on rigorous structural analysis. The models used incorporate all major components, i.e., casing-cement-formation so that all possible interactions are accounted for during modeling. Furthermore, this research shows that tensile strength is very critical for the performance of the well. Consequently, enhancing the tensile strength of well cements is an important part of this program. Some of the fiber reinforced cements tested thus far appear very promising for enhancing tensile capacity. Durability tests on fiber reinforced cements were also performed to examine corrosion characteristics and long term mechanical properties. In order to validate the effectiveness of fiber reinforcement of well cements, several comparative evaluations were made between the response of fiber reinforced and conventional cements. Essentially, two fundamental types of failures are of interest, namely, tensile failure for weak far-field stresses and shear failure in the presence of compressive far-field stresses. Similarly, stresses due to local tectonic regimes can lead to debonding of the cement annulus from the surrounding formation. The two fundamental failure modes are being investigated to see their relevance to cement mechanical properties. Interface type potential failure conditions will be considered during future work. Meanwhile, tensile and shear failure conditions were modeled by detailed finite element analysis. These numerical evaluations utilize the descriptive material models for fiber reinforced and lightweight cements determined experimentally. There is an apparent need for optimum cement formulations for all operating conditions and any transient loadings experienced by the well during its design life. This program will tackle these issues, including material behavior at elevated temperatures associated with geothermal wells.

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

HYDROGEN, FUEL CELLS & INFRASTRUCTURE TECHNOLOGIES PROGRAM

	FY 2002
HYDROGEN, FUEL CELLS & INFRASTRUCTURE TECHNOLOGIES PROGRAM - GRAND TOTAL	$815,000
FUEL CELL MATERIALS PROGRAM	$815,000
Carbon Composite Bipolar Plates for PEM Fuel Cells	200,000
Cost-Effective Metallic Bipolar Plates Through Innovative Control of Surface Chemistry	200,000
Nanopore Inorganic Membranes as Electrolytes in Fuel Cells	215,000
Metallized Bacterial Cellulose Membranes in Fuel Cells	200,000

HYDROGEN, FUEL CELLS & INFRASTRUCTURE TECHNOLOGIES PROGRAM

FUEL CELL MATERIALS PROGRAM

77. **CARBON COMPOSITE BIPOLAR PLATES FOR PEM FUEL CELLS**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: T. M. Besmann (865) 574-6852

The purpose of this work is to develop a slurry-molded carbon fiber material with a carbon chemical-vapor-infiltrated (CVI) sealed surface as a bipolar plate. During this period thermal imaging was used to demonstrate flaw identification in composite material samples, significant sensitivity to delamination and surface roughness illustrated. The Iosipescu torsion measurement method was used to determine the strength of the carbon composite bipolar plate material under more realistic mechanical stress conditions. The results are indicative of a relatively torsion resistant material, particularly given the low density of the carbon composite. The stress-displacement curves indicate little delamination or other failures until ultimate failure. A dramatic improvement in wetting of the carbon composite surface with an air oxidation treatment was demonstrated. Whereas prior to oxidative treatment water appeared to have a small wetting angle on the surface of the carbon composite, after treatment water readily spread on the surface with an apparent large wetting angle. Efforts continue to support the licensee, Porvair Fuel Cell Materials, in their effort to scale-up production.

Keywords: Bipolar Plates, Carbon Composites, Fuel Cells, Manufacturing

78. **COST-EFFECTIVE METALLIC BIPOLAR PLATES THROUGH INNOVATIVE CONTROL OF SURFACE CHEMISTRY**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: M. P. Brady (865) 574-5153

The objective of this work is to develop a bipolar plate alloy that will form an electrically conductive and corrosion-resistant nitride surface layer during thermal nitridation. A model developmental nitrided Ni-50Cr wt.% alloy exhibited no discernible degradation after 1 week immersion in pH 2 sulfuric acid at 80°C and a corrosion current density of less than 1 x 10^{-6} A/cm^2 up to ~0.9V vs standard hydrogen electrode (SHE) in pH 3 sulfuric acid at 80°C. A nitrided coupon of this material accumulated 1800 h of exposure in the Los Alamos National Lab (LANL) Corrosion Test Cell (collaboration with K. Weisbrod), with resistance increases of only 0.5 mV/1000 h at the anode and 2mV/1000 h at the cathode (for comparison, 316 stainless steel exhibits resistance increases of 16 and 21 mv/1000 h, respectively). Measurements at NREL (collaboration with H. Wang) showed that the nitridation treatment significantly lowered contact resistance relative to the untreated metallic alloy, and confirmed the excellent corrosion resistance of the nitrided surface. Future work will focus on in-cell evaluation of the model nitrided Ni-50Cr alloy to determine if the excellent corrosion resistance translates to acceptable in-cell performance, as well as reducing the level of Cr and Ni needed to yield a protective Cr-nitride layer in order to meet cost goals.

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

79. **NANOPORE INORGANIC MEMBRANES AS ELECTROLYTES IN FUEL CELLS**
$215,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
U. of Wisconsin Contact: M. A. Anderson (608) 262-2674

The objective of this work is to develop microporous inorganic oxide-based membranes of TiO_2 with high proton conductivity that are capable of operating at temperatures above 100°C with minimal water management problems. Inorganic PEMs represent a fundamental departure from the polymer-based PEMs currently used in hydrogen fuel cells. Therefore, fuel cells built using inorganic PEMs will require a significantly different fabrication method. In particular, inorganic PEMs are not free standing, but rather need to be supported on a strong, porous substrate because the membranes are inherently ultra-thin and brittle. Inorganic membranes were developed that demonstrated proton conductivity at temperatures up to 130°C at relative humidities of 81 percent. In addition, a first-generation test apparatus was fabricated to measure the performance of POEMs and MEAs containing POEMs in a functional fuel cell configuration.

Keywords: Fuel Cells, Inorganic Membranes, Proton Conductivity, PEM

80. **METALLIZED BACTERIAL CELLULOSE MEMBRANES IN FUEL CELLS**
$200,000
DOE Contact: N. L. Garland (202) 586-5673
ORNL Contact: D. P. Stinton (865) 574-4556
ORNL Principal Investigator: H. O'Neill (865) 574-5004

The objective of this task is to develop low-cost bacterial cellulose membranes with high proton conductivity that are capable of operating at above 120°C with minimal water management problems. The present concept proposes a cellulose matrix secreted by bacteria as a suitable material for PEM fuel cell technology development. The catalyst and electrolyte membrane components of the MEA are constructed using bacterial cellulose, underlining the multifunctional nature of this material. The main impact, at the system level, of a cellulose-based PEM fuel cell is that it will operate at temperatures near 130°C, circumventing the problems associated with Nafion-based PEM fuel cells. Several strategies were employed during the year to modify bacterial cellulose with ion-exchange groups. Modification of the native bacterial cellulose with phosphate groups was the most successful. Cellulose phosphate had a 2.7-fold greater thermal stability and a 7.6-fold low H_2 permeability than Nafion 117. Further characterization of this material is still required and will be carried out in conjunction with testing of the material in a membrane electrode assembly.

Keywords: Fuel Cells, Membranes, Bacterial Cellulose, Water Management

INDUSTRIAL TECHNOLOGIES PROGRAM

	FY 2002
INDUSTRIAL TECHNOLOGIES PROGRAM - GRAND TOTAL	$28,167,398
ALUMINUM VISION TEAM	$10,874,792
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$5,981,279
Innovative Vertical Floatation Melter (VFM)	800,000
Inert Metal Anode Life in Low Temperature Aluminum Reduction Process	1,190,000
Intelligent Potroom Operation	583,000
Development of a Novel Non-consumable Anode for Electrowinning Primary Aluminum	381,000
Potlining Additives	493,000
Reduction of Oxidative Melt Loss of Aluminum	531,000
Selective Adsorption of Salts from Molten Aluminum	55,000
Aluminum Carbothermic Technology	999,890
Wetted Cathodes for Low Temperature Smelting	452,000
High Efficiency Low Dross Combustion System	371,000
A Bubble Probe for Optimization of Bubble Distribution and Minimization of Splashing/Droplet Formation	100,000
Microwave Assisted Electrolytic Cell	25,389
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,513,303
Integrated Numerical Methods and Design Provisions for Aluminum Structures	93,000
Textures in Aluminum Alloys	308,000
Reduction of Annealing Times for Energy Conservation in Aluminum Processing	80,000
Surface Behavior of Aluminum Alloys Deformed under Various Processing Conditions	100,000
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	100,000
Numerical Modeling of Transient Melt Flows and Interface Instability in Aluminum Reduction Cells	28,000
Low Temperature Reduction of Alumina Using Fluorine Containing Ionic Liquids	28,000
Effect of Impurities on the Processing of Aluminum Alloys in Casting, Extrusion, and Rolling	22,303
Combined Experimental and Computational Approach for the Design of Mold Surface Topography	28,000
Molten Aluminum Treatment by Salt Fluxing with Low Environmental Emissions	21,000
Inert Metal Anodes for Primary Aluminum Production	220,000
Improved Energy Efficiency in Aluminum Melting	765,000
Evaluation and Characterization of In-Line Annealed Continuous Cast Aluminum Sheet	520,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,380,210
Processing and Recycling of Aluminum Wastes	111,000
Wettable Ceramic-based Drained Cathode Technology for Aluminum Electrolysis Cells	720,000
Spray Rolling Aluminum Strip	133,000
Modeling Optimization of Direct Chill Casting	404,000
Degassing of Aluminum Alloys Using Ultrasonic Vibrations	60,000
Effect of Casting Conditions & Composition on Microstructural Gradients in Roll Cast Aluminum Alloys	30,010
Energy Efficient Isothermal Melting of Aluminum	479,000
Coolant Characteristics and Control in Direct Chill Casting of Aluminum	130,000
Continuous Severe Deformation Processing of Aluminum Alloys	300,000
Development of a Rolling Process Design Tool for Use in Improving Hot Roll Slab Recovery	13,200

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2002
GLASS INDUSTRY OF THE FUTURE	$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
FOREST AND PAPER PRODUCTS	$1,950,792
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$615,000
Particle Formation and Deposition in Recovery Boiler Applications	270,000
Non-Process Element (NPE) Removal Using Functionalized Monolayers on Mesoporous Supports	280,000
Use of Residual Solids From Pulp and Paper Mills for Enhancing Strength and Durability of Ready-Mixed Concrete	65,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,335,792
Corrosion in Kraft Digesters: Characterization and Evaluation of Corrosion Control Methods	599,542
Selection and Development of Refractory Structural Materials for Black Liquor Gasification	200,000
Chromium Rich Alloys for Gasifier and Kraft Recovery Boiler Applications	247,500
Ceramic Coatings for Use in High Temperature, High Pressure Black Liquor Gasifiers	288,750
METAL CASTING	$1,403,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$439,000
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	63,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$964,000
Clean Cast Steel: 1) Machinability of Cast Steel; 2) Accelerated Transfer of Clean Steel Technology	166,000
Prevention of Porosity in Iron Castings	47,000
Advanced Lost Foam Casting Technology	218,000
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	107,000
Improvements in Sand Mold/Core Technology: Effects on Casting Finish	106,000
Heat Checking and Washout of Superalloys for Die Inserts	100,000

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2002
INDUSTRIAL MATERIALS FOR THE FUTURE	$13,738,814
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING	$9,096,676
Advanced Materials/Processes	1,090,000
Conducting Polymers: Synthesis and Industrial Applications	150,000
Development of Advanced Metallic/intermetallic Alloys	670,000
High Temperature Facilitated Membranes	350,000
Intermetallic Alloy Development and Technology Transfer of Intermetallic Alloys	2,458,000
Plasma Processing-Advanced Materials for Corrosion and Erosion Resistance	300,000
Development of Ultrananocrystalline Diamond (UNCD) Coatings for SiC Multipurpose Mechanical Pump	250,000
Exploring Ultrahigh Magnetic Field Processing of Materials for Developing Customized Microstructures and Enhanced Performance	200,000
Inverse Process Analysis for the Acquisition of Accurate Thermophysical Data	250,000
Development of Stronger and More Reliable Cast Austenitic Stainless Steels	300,000
Ultrasonic Processing of Materials	150,000
High Energy Density Coating of High Temperature Advanced Materials for Energy Efficient Performance	150,000
Novel Carbon Films for next Generation Rotating Equipment Applications	225,676
Advanced Composite Coatings	300,000
High-Density Infrared Surface Treatments of Refractories	200,000
Development of a New Class of Ferritic Steels for Industrial Process Applications	500,000
Crosscutting Industrial Applications of a New Class of Ultrahard Borides	245,000
Development of Advanced Wear and Corrosion Resistant Systems Through Laser Surface Alloying and Materials Simulation	170,000
Development and Demonstration of Advanced Tooling Alloys for Molds and Dies	180,000
Novel Superhard Materials and Nanostructured Diamond Composites	358,000
Advanced Nanoporous Composite Materials for Industrial Heating Applications	300,000
High Density Infrared (HDI) Transient Fused Coatings for Improved Wear and Corrosion Resistance	300,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,937,182
Materials Development for the Forest Products Industry	400,000
Metals Processing Laboratory Users (MPLUS) Facility	1,000,000
Development of Combinatorial Methods for Alloy Design and Optimization	200,000
Stochastic Multi-Objective Optimization of Heat and Corrosion Resistant Alloy Properties	186,617
Fracture Toughness and Strength in a New Class of Bainitic Chromium Tungsten Steels	124,000
Characterization and Structural Modeling of Magnesia-alumina Spinel Refractories	300,565
Thermochemical Models High-temperature Materials Processing and Corrosion	200,000
Virtual Weld-Joint Design Integrating Advanced Materials and Processing Technologies	250,000
Stress-Assisted Corrosion (SAC) in Boiler Tubes	276,000
MATERIALS STRUCTURE AND COMPOSITION	$300,000
Development of Cost-effective Low Permeability Ceramic and Refractory Components for Aluminum Melting and Casting	300,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,404 ,956
Continuous Fiber Ceramic Composites (CFCC) - Industrial Technologies	750,000
Selective Inorganic Thin Films	250,000
Physical and Numerical Analysis of Extrusion Process for Production of Bimetallic Tubes	200,000
High Performance, Oxide Dispersion Strengthened Tubes for Production of Ethylene	204,956

INDUSTRIAL TECHNOLOGIES PROGRAM

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

81. **INNOVATIVE VERTICAL FLOATATION MELTER (VFM)**
$800,000
DOE Contact: Tom Robinson (202) 586-0139

The Energy Research Company, O'Brien & Gere Engineers, Inc., and Stein, Atkinson Stordy Ltd. are project partners for the development of VFM. Recycled aluminum accounts for more than one third of the total U.S. aluminum supply. Aluminum recycling results in significant energy savings, lower emissions and an increase in metal yield. Typically, aluminum scrap is cleaned/decoated and then melted in gas reverberatory furnaces that have low thermal efficiencies (20%) and generate substantial emissions. The vertical floatation melter is an innovative design that decoats, preheats and melts in one operation. The pilot demonstrated design provides a thermal efficiency of 58%. Not only is energy saved, but also the emissions are significantly reduced and more metal is recovered. The design provides a higher metal yield (dross reduction) because of lower gas temperature, lower residence time, lower oxygen content and no direct flame impingement on the metal. The VFM is a versatile design that can be integrated with indirect-fired controlled-atmosphere rotating kilns. This integration provides additional savings, with thermal efficiencies of over 75 percent in recovering aluminum scrap. This process also has applications in the glass and steel industries. A pilot scale unit capable of processing 1,000 pounds per hour of aluminum has been designed, constructed and successfully tested. Pilot operations have demonstrated a thermal efficiency (the ratio of heat going into scrap aluminum to that of the total energy used) of more than 2.5 times that of a conventional furnace, lower emissions and improved metal recovery (dross reduced by more than half). This project has now entered the planning, site preparation and field-testing phase that will demonstrate the VFM's commercial use.

Keywords: Floatation Melter, Aluminum Scrap

82. **INERT METAL ANODE LIFE IN LOW TEMPERATURE ALUMINUM REDUCTION PROCESS**
$1,190,000
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^{o}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

83. **INTELLIGENT POTROOM OPERATION**
$583,000
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

84. **DEVELOPMENT OF A NOVEL NON-CONSUMABLE ANODE FOR ELECTROWINNING PRIMARY ALUMINUM**
$381,000
DOE Contact: Tom Robinson (202) 586-0139

Ohio State University assisted by Gas Research Institute, Kaiser Aluminum, Siemens-Westinghouse and TDA Research are project partners for the development of a novel non-consumable anode. Since the patenting of the Hall-Héroult Cell (HHC) in 1886 for electrowinning aluminum, the basic features have remained essentially the same. Although significant optimization has occurred, industry acknowledges that there are many problems associated with the use of the consumable carbon anode. This project is developing a novel non-consumable (gas) anode that will displace today=s carbon anode (eliminating the carbon plant), and serve as a retrofit into the current HHC. The anode is comprised of a thin, dense oxide-ion-conducting membrane with an electrocatalytic porous internal anode where reformed natural gas is electrochemically oxidized. Application of such a non-consumable anode retrofitted into the HHC would significantly increase the energy efficiency, reduce the emissions, and reduce the cost of producing primary aluminum compared to the best current and emerging anode replacement technologies.

Keywords: Carbon Anode, Aluminum Production, Smelting

85. **POTLINING ADDITIVES**
$493,000
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

86. **REDUCTION OF OXIDATIVE MELT LOSS OF ALUMINUM**
$531,000
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

87. **SELECTIVE ADSORPTION OF SALTS FROM MOLTEN ALUMINUM**
$55,000
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

88. **ALUMINUM CARBOTHERMIC TECHNOLOGY**
$999,890
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

89. **WETTED CATHODES FOR LOW TEMPERATURE SMELTING**
$452,000
DOE Contact: Tom Robinson (202) 586-0139

Wetted cathodes and inert anodes have potentially significant advantages over the century old Hall-Héroult cell used today for worldwide aluminum production. Wetted cathodes allow for decreased anode-cathode distances accompanied by reduced voltages and energy consumption. Inert anode replacement of conventional carbon anodes will eliminate the emission of greenhouse gases associated with the production of primary aluminum (e.g., CO, CO_2 and perfluorocarbons) and with the manufacture of the carbon anodes. The use of wettable cathodes with inert anodes could reduce the energy needed for primary aluminum production by 25 to 30 percent. The adoption of these advanced electrodes has been hindered by their rapid corrosion, particularly of the cathode, when operating at a conventional temperature of 950°C. A low temperature electrolysis (LTE) cell that operates about 200°C lower than a conventional cell offers a more benign environment for advanced electrodes. This project will extend the knowledge of wetted cathode operation and failure mechanisms. It will prepare and screen various wetted cathode materials for aluminum LTE cells and develop techniques to measure and evaluate the aluminum film on the wetted cathode. Successful development of this technology will lower both capital and operating costs and offer many advantages in energy and environmental conservation. Project partners include Northwest Aluminum Technologies, assisted by Advanced Refractory Technologies, Material Modification Inc., Electrochemical Technology Corp., Brooks Rand Limited, and Pacific Northwest National Laboratory.

Keywords: Low Temperature Electrolysis, Inert Anode, Wetted Cathode

90. **HIGH EFFICIENCY LOW DROSS COMBUSTION SYSTEM**
$371,000
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

91. **A BUBBLE PROBE FOR OPTIMIZATION OF BUBBLE DISTRIBUTION AND MINIMIZATION OF SPLASHING/ DROPLET FORMATION**
$100,000
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

92. **MICROWAVE ASSISTED ELECTROLYTIC CELL**
$25,389
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

93. **INTEGRATED NUMERICAL METHODS AND DESIGN PROVISIONS FOR ALUMINUM STRUCTURES**
$93,000
DOE Contact: Tom Robinson (202) 586-0139

Project partners for this research effort are the Aluminum Association and Cornell University. Aluminum’s competitive edge arises from the ease with which shapes can be extruded. Yet, this advantage cannot be fully exploited by designers because they do not have the tools to predict the strength of many extrudable shapes. Suggested specifications for the structural design of parts made of various aluminum alloys were developed in 1962 and published in 1967 in Specifications for Aluminum Structures (Aluminum Association). The document has been revised five times, most recently in 1994, but methods for determining the buckling strength of extrusions are essentially unchanged. Many types of stiffeners, such as web stiffeners and multiple intermediate stiffeners, thickness changes and other cross-sectional peculiarities cannot be addressed by the current specification even though they add significantly to the load carrying capacity. Researchers from Cornell University will develop and demonstrate a design methodology using finite strip analysis. It will result in design rules applicable to many extrudable or cold-rolled shapes. Columns, beams, and beam columns will be studied. A wide variety of failure modes such as local, distortional, torsional, torsional-flexural, and lateral buckling will be researched. Failures involving the interaction of these modes, such as the local and overall buckling will be included in the study as well.

Keywords: Aluminum Extrusions, Aluminum Structures, Design Provisions

94. **TEXTURES IN ALUMINUM ALLOYS**
$308,000
DOE Contact: Tom Robinson (202) 586-0139

Aluminum sheets made by continuous strip casting provide energy savings of greater than 26 percent and cost savings of more than 19 percent compared to sheets made from ingot casting and rolling. Sheet formability is among the most important characteristics of aluminum sheet. Formability depends on the crystal grain structure and is a result of the casting method and processing sequences used to produce the sheet. The demand for aluminum sheets is increasing particularly in the transportation industry where they are used to produce lighter, more fuel-efficient vehicles. As more complex forms are required, improved process controls are needed. Industry currently relies on post-processing testing to determine formability characteristics of finished sheet. The on-line monitoring of the continuously cast sheet production process will allow simultaneous control of important forming parameters. Crystallographic texture is related to the mechanical anisotropy/formability of metallic sheets. University of Kentucky and Commonwealth Aluminum will determine if there is a quantitative relationship between crystallographic texture measurements at processing temperatures and aluminum sheet formability. Data will be collected from two different spectroscopic measuring devices. This data will then be analyzed to determine if these instruments can produce measurements of the formability characteristics. The instrument proven to be most effective for measuring texture and formability at processing temperatures will be installed on-line in a production facility to demonstrate the ability to measure and control formability in continuous strip production.

Keywords: Textures in Aluminum Alloys, Crystallographic, Continuous Casting

95. **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

96. **SURFACE BEHAVIOR OF ALUMINUM ALLOYS DEFORMED UNDER VARIOUS PROCESSING CONDITIONS**
$100,000
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

97. **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

98. **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

99. **DEVELOPMENT OF INTEGRATED METHODOLOGY FOR THERMO-MECHANICAL PROCESSING OF ALUMINUM ALLOYS**
$100,000
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

100. **NUMERICAL MODELING OF TRANSIENT MELT FLOWS AND INTERFACE INSTABILITY IN ALUMINUM REDUCTION CELLS**
$28,000
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

101. **LOW-TEMPERATURE REDUCTION OF ALUMINA USING FLUORINE CONTAINING IONIC LIQUIDS**
$28,000
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

102. **EFFECT OF IMPURITIES ON THE PROCESSING OF ALUMINUM ALLOYS**
$22,303
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

103. **COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACH FOR THE DESIGN OF MOLD SURFACE TOPOGRAPHY**
$28,000
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

104. **MOLTEN ALUMINUM TREATMENT BY SALT FLUXING WITH LOW ENVIRONMENTAL EMISSIONS**
$21,000
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

105. **INERT METAL ANODES FOR PRIMARY ALUMINUM PRODUCTION**
$220,000
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

106. **IMPROVED ENERGY EFFICIENCY IN ALUMINUM MELTING**
$765,000
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

107. **EVALUATION AND CHARACTERIZATION OF IN-LINE ANNEALED CONTINUOUS CAST ALUMINUM STEEL**
$520,000
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

108. **PROCESSING AND RECYCLING OF ALUMINUM WASTES**
$111,000
DOE Contact: Tom Robinson (202) 586-0139

This project at Michigan Technological University focuses on the development of a technology to divert the salt cake into valuable feedstock materials for the manufacturing of concrete products such as lightweight masonry, foamed concrete, and mine backfill grouts. By using the unique properties inherent in the aluminum salt cake, this by-product can function as a foaming (air entraining) agent, and fine aggregate for use in concrete. The technology is expected to benefit the aluminum, concrete, mining and construction industries. The aluminum industry will be able to increase its recovery of aluminum metal while reducing energy consumption. Technology development objectives include:

- Process by-product waste streams from several aluminum smelters and optimizes the processing required to convert wastes into products suitable for use as concrete additives.
- Develop and demonstrate the processing required to effectively utilize the processed by-products developed for the production of mine backfill grouts.
- Develop and demonstrate the processing required for lightweight aggregate/masonry block production utilizing the processed by-products developed.
- Document the environmental acceptability of the smelting by-products used as concrete additives and assess the environmental acceptability of the low-density concrete products made using these additives.

Keywords: Salt Cake, Recycling, Feedstock, Waste Streams, Concrete Additives

109. **WETTABLE CERAMIC-BASED DRAINED CATHODE TECHNOLOGY FOR ALUMINUM ELECTROLYSIS CELLS**
$720,000
DOE Contact: Tom Robinson (202) 586-0139

Reynolds Metals Company, Kaiser Mead, and Advanced Refractory Technologies (ART) will collaborate to develop and evaluate ceramic-based materials, technology, and the necessary engineering packages to retrofit existing reduction cells as a means to improve the performance of the Hall Héroult cell. ART will produce TiB_2-based tiles or coatings that will be used as the "drained" lining in two 70 kA prebake cells. The durability of the candidate materials and the performance of the drained cathode design will be evaluated during a one-month test using 12 kA pilot reduction cells. This four-year project, initiated in September 1997, will include the following activities:

- Development and evaluation of candidate TiB_2 carbon materials (tiles and coating)
- Development and evaluation of proprietary carbon materials
- Development of the drained cathode design
- Evaluation of the best candidate materials and the drained cathode design in the 12 kA pilot cell
- Design and construction of a 70 kA prebake cell retrofitted with a drained cathode using TiB_2-based and or the proprietary materials
- Startup and operation of two 70 kA prebake cells retrofitted with a drained cathode and TiB_2 and or the proprietary materials

Keywords: Cathode, Aluminum Production, Titanium Diboride

110. **SPRAY ROLLING ALUMINUM STRIP**
$133,000
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

111. **MODELING OPTIMIZATION OF DIRECT CHILL CASTING**
$404,000
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

112. **DEGASSING OF ALUMINUM ALLOYS USING ULTRASONIC VIBRATIONS**
$60,000
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

113. **EFFECT OF CASTING CONDITIONS AND COMPOSITION ON MICROSTRUCTURAL GRADIENTS IN ROLL CAST ALUMINUM ALLOYS**
$30,010
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

114. **ENERGY EFFICIENT ISOTHERMAL MELTING OF ALUMINUM**
$479,000
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

115. **COOLANT CHARACTERISTICS AND CONTROL IN DIRECT CHILL CASTINGS OF ALUMINUM**
$130,000
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

116. **CONTINUOUS SEVERE PLASTIC DEFORMATION PROCESSING OF ALUMINUM ALLOYS**
$300,000
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

117. **DEVELOPMENT OF A ROLLING PROCESS DESIGN TOOL FOR USE IN IMPROVING HOT ROLL SLAB YIELD**
$13,200
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 INDUSTRY OF THE FUTURE

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) 5861476.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

118. **DEVELOPMENT OF MODELS AND ON-LINE DIAGNOSTIC MONITORS OF THE HIGH-TEMPERATURE CORROSION OF REFRACTORIES IN OXY-FUEL GLASS FURNACES**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936
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 FY02 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

FOREST AND PAPER PRODUCTS

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

119. **PARTICLE FORMATION AND DEPOSITION IN RECOVERY BOILER APPLICATIONS**
$270,000
DOE Contact: David Boron (202) 586-0080
SNL Contact: Christopher R. Shaddix (925) 294-3840
Brigham Young University Contact: (801) 378-8616

The initial objective of this project was to measure the rate of ash deposit accumulation, and the properties of such deposits, under convection pass conditions in a recovery boiler. A follow-on objective is to quantify the concentration of intermediate-size particles (ISPs) entrained in typical recovery boilers, identify the mechanisms and rates of intermediate-size particle formation and deposition, and propose means of controlling their impact on boiler operation. This is a seven-year project with an expected completion date of September 30, 2003.

Keywords: Deposition, Particle Formation, Recovery, Boilers

120. **NON-PROCESS ELEMENT (NPE) REMOVAL USING FUNCTIONALIZED MONOLAYERS ON MESOPOROUS SUPPORTS**
$280,000
DOE Contact: Dickson Ozokwelu (202) 586-8501
PNNL Contact: Robert Leugemors (509) 372-2814

The goal of this project is to develop extremely high capacity, high selective sorbent materials to remove non-process elements (NPEs) from bleach cycle filtrate and facilitate the partial or complete closure of the waste water stream in modern kraft mill bleaching plants. Experiments will focus on the synthesis of functionalized mesoporous materials (SAMMS) specifically designed to remove three general classes of NPEs: namely alkaline earth cations (Ca, Ba, Mg), transition metal cations (Mn, Fe, Cu), and certain problematic anions (PO_4, silicate aluminate, phenolate). This is a three year project with an expected completion date of September 30, 2002.

Keywords: Removal, Synthesis, Mesoporous Materials

121. **USE OF RESIDUAL SOLIDS FROM PULP AND PAPER MILLS FOR ENHANCING STRENGTH AND DURABILITY OF READY-MIXED CONCRETE**
$65,000
DOE Contact: Dickson Ozokwelu (202) 586-8501
University of Wisconsin - Milwaukee Contact: Tarun R. Naik (414) 299-6696

This project will develop a new type of ready-mixed concrete using fibrous residuals from pulp and paper mill primary effluent sludge. The project will provide a practical solution to disposal problems for pulp and paper mill byproducts and provide an economical source of fiber reinforcement for ready mixed concrete production. The varying lengths of fibers available from pulp and paper mill sludge will help improve the tensile, flexural and compressive strength of the concrete. This is a four year project with an expected completion date of December 31, 2003.

Keywords: Pulp and Paper, Byproducts, Concrete

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

122. **CORROSION IN KRAFT DIGESTERS: CHARACTERIZATION AND EVALUATION OF CORROSION CONTROL METHODS**
$599,542
DOE Contact: David Boron (202) 586-0080
ORNL Contact: James Keiser (865) 574-4453

This project will correlate chemical pulping digester conditions with material performance. Digester conditions will be evaluated using a computational fluid dynamics model of flow with a digester. This flow model will be supplemented with a model for the chemical reactions occurring in the digester. *In situ* and laboratory corrosion studies will be used to provide information about the corrosion behavior of conventional materials. An assessment of corrosion control methods and alternative materials will be performed. This is a five-year project with an expected completion date of September 30, 2003.

Keywords: Digester, Corrosion, Pulp and Paper

123. **SELECTION AND DEVELOPMENT OF REFRACTORY STRUCTURAL MATERIALS FOR BLACK LIQUOR GASIFICATION**
$200,000
DOE Contact: David Boron (202) 586-0080
ORNL Contact: James Keiser (865) 574-4453

This project will identify refractory materials that have acceptable life to allow gasifiers to effectively and economically operate using black liquor or biomass feedstocks. Working with industrial partners, the investigators will identify and address the most serious material problems associated with the top three emerging biomass and black liquor gasification technologies. Studies will be performed to identify or develop more suitable materials for these applications. This is a four year project with an expected completion date of September 30, 2003.

Keywords: Gasification, Black Liquor, Refractory, Pulp and Paper

124. **CHROMIUM-RICH ALLOYS FOR GASIFIER AND KRAFT RECOVERY BOILER APPLICATIONS**
$247,500
DOE Contact: David Boron (202) 586-0080
ORNL Contact: Micheal P. Brady (865) 574-5153

This project is an effort to develop a new family of molten smelt resistant chromium-rich alloys with sufficient ductility and toughness to permit use as structural components and/or coatings for gasifier and recovery boiler applications. The project will significantly leverage experience and laboratory scale molten salt testing infrastructure gained in previous efforts for recovery boiler materials and refractory materials for gasifiers. This is a three year project with an expected completion date of September 30, 2004.

Keywords: Gasification, Recovery, Boilers

125. **CERAMIC COATINGS FOR USE IN HIGH TEMPERATURE, HIGH PRESSURE BLACK LIQUOR GASIFIERS**
$288,750
DOE Contact: David Boron (202) 586-0080
ORNL Contact: James R. Keiser (865) 574 4453

The primary objective of this project is to identify at least one ceramic/refractory material that has the appropriate thermal conductivity, smelt corrosion resistance and thermal shock resistance to serve as a thermal and chemical protective layer on a water-cooled metal tube in a high-temperature, high-pressure black liquor gasifier. Alternatively, if it can be demonstrated that a metal tube can be fabricated that is resistant to this environment, then that formation will be provided to the designers. In either case, this constraint on gasifier development would be eliminated. This is a three year project with an expected completion date of 9/30/04

Keywords: Ceramics, Refractory, Black Liquor, Gasification

METAL CASTING

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

126. **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 4,500psi 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

127. **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

128. **INTEGRATION OF RSP TOOLING WITH RAPID PROTOTYPING FOR DIE-CASTING APPLICATION**
$63,000
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

129. **CLEAN CAST STEEL: 1) MACHINABILITY OF CAST STEEL; 2) ACCELERATED TRANSFER OF CLEAN STEEL TECHNOLOGY**
$166,000
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

130. **PREVENTION OF POROSITY IN IRON CASTINGS**
$47,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
Climax Research Services Contact: James Lakin
(248) 960-4900, Ext. 210

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

131. **ADVANCED LOST FOAM CASTING TECHNOLOGY**
$218,000
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

132. **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

133. **FERRITE MEASUREMENTS IN DUPLEX STAINLESS STEEL CASTINGS**
$120,000
DOE Contact: Ehr Ping HuangFu (202) 586-1493
University of Tennessee Contact: Carl Lundin (865) 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

134. **TECHNOLOGY FOR THE PRODUCTION OF CLEAN, THIN WALL, MACHINABLE GRAY AND DUCTILE IRON CASTINGS**
$107,000
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

135. **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

136. **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 nickel 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

INDUSTRIAL MATERIALS FOR THE FUTURE

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 effort and of crosscutting industries including the carbon products, forging, heat treating, process heating, and welding industries. Efforts in FY 2002 were focused on development of the new IMF program plan and issuing proposals related to the industry, academia, and national laboratory sectors. The DOE program managers are Sara Dillich (202) 586-7925 and Mike Soboroff (202) 586-4936.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING

137. **ADVANCED MATERIALS/PROCESSES**
$1,090,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goals of this project are to develop new and improved materials and materials processing methods. Metallic, intermetallic alloys, refractories and ceramics possess unique properties and have the potential to be developed as new materials for energy related applications. In FY 2001, R&D also utilized the new 300,000 W high intensity infrared heating and processing system. Research conducted related to surface modification of ceramics, refractory and alloy systems, materials properties, thermodynamics, and high temperature filtration materials.

Keywords: Intermetallic, Metalcasting, Glass, Alloys, Welding, Corrosion Resistance, Infra Red Heating, Coatings, Refractories, WC, Thermodynamics, Materials Properties, Thermal Spray, Ceramics, Materials Processing

138. **CONDUCTING POLYMERS: SYNTHESIS AND INDUSTRIAL APPLICATIONS**
$150,000
DOE Contact: Mike Soboroff (202) 586-4936
Los Alamos National Laboratory Contact: S. Gottesfeld (505) 667-0853

In FY 2001, the use of conducting polymers for electrochemical reactors (ECRs) based on polymeric electrolytes was addressed. The objective of this effort is to develop and test electrochemical reactors for the chlor-alkali industry, based on polymer membrane/electrode assemblies and on oxygen or air electrodes. In FY 2001, development of the oxygen polarized chlor-alkali cells was continued.

Keywords: Electrically Conducting Polymers, Gas Separation, Electrochemical Reactors, Cathodes

139. **DEVELOPMENT OF ADVANCED METALLIC/INTERMETALLIC ALLOYS**
$670,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contacts: P. J. Maziasz (865) 574-5082, M. L. Santella (865) 574-4805, V. K. Sikka (865) 574-5112 and C. T. Liu (865) 574-4459

The objectives of this project are to develop advanced intermetallic alloys including FeAl and Ni_3Si. The FeAl effort is focused on alloys with improved weldability and mechanical and corrosion properties for use in structural applications; and the development of weldable FeAl alloys for use in weld-overlay cladding applications. The Ni_3Si effort is focusing on alloy composition, and welding. Developments made in FY 2001 included;
1) improvement of the ductility and joining of nickel silicide, 2) development of autogenous and dissimilar metal welding of iron aluminide, and 3) corrosion studies in carburizing environments.

Keywords: Iron Aluminides, Nickel Aluminides, Coatings, Claddings, Thermophysical Properties, Casting, Thermomechanical Properties, Chemical Industry, Steel Industry, Welding, Alloys, Intermetallic, Joining

140. **HIGH TEMPERATURE FACILITATED MEMBRANES**
$350,000
DOE Contact: Mike Soboroff (202) 586-4936
Los Alamos National Laboratory: D. J. Devlin (505) 667-9914

The project focuses on the development of membranes and a test system for their evaluation. The purpose of the project is to develop and evaluate a new high-temperature membrane for the separation of carbon dioxide from hydrogen. The approach involves the use of molten carbonate type materials with reversibility, measurement of transport properties through membranes, and the evaluation of decomposition to oxide on the downstream side. In FY2001, progress was made in fabricating membranes of lithium carbonate on metallic substrates.

Keywords: Membranes, Liquid Vapor Separations, Oxygen, Carbon Dioxide, Natural Gas, Corrosion

141. **INTERMETALLIC ALLOY DEVELOPMENT AND TECHNOLOGY TRANSFER OF INTERMETALLIC ALLOYS**
$2,458,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contacts: M. L. Santella (865) 574-4805 and V. K. Sikka (865) 574-5112
University of Tennessee Contact: G. M. Pharr (865) 974-8202

The objective of this project is to develop and apply the excellent oxidation and carburization resistance and higher strength of intermetallic alloys including nickel aluminides to Industries of the Future related manufacturing applications. Progress in bringing technologies to development and commercialization in FY 2000 included: 1) processing of radiant tubes and rolls for testing and evaluation, 2) the evaluation of long term stability tests of nickel aluminide, and 3) joining technology for the iron aluminide system.

Keywords: Nickel Aluminides, Processing, Steel, Metalcasting, Heat Treating, Welding, Chemical Properties, Intermetallic, Alloys, Joining

142. **PLASMA PROCESSING - ADVANCED MATERIALS FOR CORROSION AND EROSION RESISTANCE**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936
Los Alamos National Laboratory: M. Trkula (505) 667-0591

The project focuses on developing coating technologies to obtain erosion, and corrosion resistant, thermo-dynamically stable, and adherent coatings on die materials used to cast aluminum and other metals. Low temperature organo-metallic chemical vapor deposition combined with immersion ion processing is being developed as the coating technology. In FY 2001, various coatings were produced on substrates and evaluated.

Keywords: Plasma, Processing, Corrosion, Erosion, Coatings, Materials, Metals

143. **DEVELOPMENT OF ULTRANANOCRYSTALLINE DIAMOND (UNCD) COATINGS FOR SiC MULTIPURPOSE MECHANICAL PUMP**
$250,000
DOE Contact: Mike Soboroff (202) 586-4936

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. The commercialization of UNCD-based seals will require development of microwave plasma chemical vapor deposition tools for growing high quality, cost efficient UNCD coatings.

Keywords: Coatings, Chemical Vapor Deposition, Ultrananocrystalline Diamond

144. **EXPLORING ULTRAHIGH MAGNETIC FIELD PROCESSING OF MATERIALS FOR DEVELOPING CUSTOMIZED MICROSTRUCTURES AND ENHANCED PERFORMANCE**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

Demonstrate and document the influence of ultrahigh magnetic field processing on the phase equilibria in ferrous alloys. The principal objective 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 Since essentially all materials have some form of ferromagnetism or paramagnetism, magnetic field processing is directly applicable to a multitude of materials for dramatically influencing phase stability and phase transformation kinetics through appropriate selection of magnetic field strength promises to provide a very robust mechanism to develop and tailor microstructures for a broad spectrum of materials applications. Ferrous alloys will be 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

145. **INVERSE PROCESS ANALYSIS FOR THE ACQUISITION OF ACCURATE THERMOPHYSICAL DATA**
$250,000
DOE Contact: Mike Soboroff (202) 586-4936

The goal of this project is to improve the acquisition of data on thermophysical properties (including 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 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 Develop analytical models for DSC, Develop analytical models for dilatometry, Conduct DSC and dilatometry measurements, Experimentally validate the proposed methodologies, and Evaluate and summarize experimental and computational procedures.

Keywords: Dilatometry, Thermophysical Properties, DSC

146. **DEVELOPMENT OF STRONGER AND MORE RELIABLE CAST AUSTENITIC STAINLESS STEELS**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goal of this project is to increase the high-temperature creep strength by 50% 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 will focus on the use of alloy design methods developed at the 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.

Keywords: Steel, Microstructure Properties, Alloys

147. **ULTRASONIC PROCESSING OF MATERIALS**
$150,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goals of the project are to evaluate the core principles, establish a quantitative basis for the ultrasonic processing of materials, and to demonstrate key applications in the areas of 1) grain refinement of alloys during solidification, and 2) degassing of alloy melts. This study will focus on two classes of materials, aluminum alloys and specialty steels, and will demonstrate the application of ultrasonic processing during ingot (and continuous) casting, foundry shape casting, and vacuum arc remelting. This investigation proposes to study the effects of acoustic energy of varying phonon energy and frequency introduced during the melting and solidification process. Acoustic frequencies from dc to 100 MHz, and continuous acoustic input power of up to 100 watts will be used. Variables will be input acoustic power, input acoustic frequency, and cooling rate.

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

148. **HIGH ENERGY DENSITY COATING OF HIGH TEMPERATURE ADVANCED MATERIALS FOR ENERGY EFFICIENT PERFORMANCE**
$150,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goal of the project is to develop a reliable, efficient, and economic method of coating ceramic on metal by using a high-energy-density technique. The process and coating-substrate material systems will be optimized to suit specific industrial applications. The goal also includes characterization of processed coating-substrate material systems for wear and corrosion properties under various conditions. The correlation between coating properties and process parameters will be established. The major objectives of the research activity are 1) to understand the chemical, physical, and microstructural transformations taking place in the selected representative systems during LPIASM treatment (this knowledge about various transformations is necessary to subsequently develop highly efficient and cost-effective customized applications for surface protection/modification) and 2) to develop a technique for modifying the surfaces of various geometries and materials for enhanced wear and corrosion properties in real components.

Keywords: Ceramic, Advanced Materials, Coatings, Wear, Corrosion

149. **NOVEL CARBON FILMS FOR NEXT GENERATION ROTATING EQUIPMENT APPLICATIONS**
$225,676
DOE Contact: Mike Soboroff (202) 586-4936

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

150. **ADVANCED COMPOSITE COATINGS**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936

The goal of the project is to develop low-cost, high-temperature corrosion-resistant coatings with superior mechanical properties for industrial applications. Two methods will be used to fabricate high-temperature corrosion resistant ceramic coatings: 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 will also be developed as a means to further improve coating performance. Composite coatings will 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

151. **HIGH-DENSITY INFRARED SURFACE TREATMENTS OF REFRACTORIES**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goal of the project is to make a major advancement in improving the behavior of refractory materials used in industrial processes. Refractories play an integral part in the operations of numerous industries of the future, and advancements can have a significant and large impact on the viability of those industries. These improvements will be realized through surface modifications with HDI. The project will be performed as a series of tasks. The objectives of the three 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).

Keywords: Infrared, Refractories, HDI, Porosity, Corrosion Resistance, Coatings, Sintering

152. **DEVELOPMENT OF A NEW CLASS OF FERRITIC STEELS FOR INDUSTRIAL PROCESS APPLICATIONS**
$500,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

Development of a new class of Fe-3Cr-W(V) steels with 1) 50% higher tensile strength at temperatures up to 650˚C than current alloys 2) potential for not requiring any PWHT 3) equipment weight reduction of 25 percent, and 4) impact properties of approximately 100 ft-lb upper shelf energy and -10˚F (-20˚C) for DBTT without tempering treatment. The project objectives will be 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, High Tensile Strength, Alloys, Thermodynamic Modeling, Welding, Mechanical Properties

153. **CROSSCUTTING INDUSTRIAL APPLICATIONS OF A NEW CLASS OF ULTRAHARD BORIDES**
$245,000
DOE Contact: Mike Soboroff (202) 586-4936
Ames Laboratory, Iowa State University Contact: Bruce Cook (515) 294-9673

The goal of this project is to develop a new class of ultrahard materials, based on the complex boride AIMgB14, 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 AIMgB14 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).

Keywords: Borides, Metalcasting, Forest Products, Mining, Agriculture, Alloys, Ductility, Fracture Toughness

154. **DEVELOPMENT OF ADVANCED WEAR AND CORROSION RESISTANT SYSTEMS THROUGH LASER SURFACE ALLOYING AND MATERIALS SIMULATION**
$170,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

Development of processing and material simulation techniques for identifying and creating reproducible advanced coatings through the LSA process. 1) Extend the laser process, computational thermodynamics and kinetic models to describe the microstructure evolution during LSA processing for well-characterized process conditions. 2) Evaluate the predictions with experimental microscopy and analysis. 3) Use the theoretical models and experimental measurements to develop new advanced composite-coating systems with collaborating industrial members.

Keywords: Coatings, Alloys, Laser Surface Alloying, Thermodynamic Models, Advanced Composites, Microscopy, Corrosion

155. **DEVELOPMENT AND DEMONSTRATION OF ADVANCED TOOLING ALLOYS FOR MOLDS AND DIES**
$180,000
DOE Contact: Mike Soboroff (202) 586-4936
Idaho National Engineering and Environmental Laboratory Contact: Kevin McHugh (208) 526-9662

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. The objectives of this effort include increasing die life by a minimum of 20 percent and reducing energy consumption associated with the manufacture and heat treatment of dies by a minimum of 25 percent.

Keywords: Alloys, Molds, Glass, Forging, Die Casting, Heat Treating

156. **NOVEL SUPERHARD MATERIALS AND NANOSTRUCTURED DIAMOND COMPOSITES**
$358,000
DOE Contact: Mike Soboroff (202) 586-4936
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 success of this project can have significant technological impacts for future industrial applications in many fields. 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.

Keywords: Diamond Composites, Superhard Materials, Nanostructure, Solvents, Catalysts, Crystallization, High Pressure Techniques, SiC

157. **ADVANCED NANOPOROUS COMPOSITE MATERIALS FOR INDUSTRIAL HEATING APPLICATIONS**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936
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. Advanced composite structures will be prepared and similarly analyzed.

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

158. **HIGH DENSITY INFRARED (HDI) TRANSIENT FUSED COATINGS FOR IMPROVED WEAR AND CORROSION RESISTANCE**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936

The project's aims are 1) to develop, evaluate, and understand how high density infrared heating technology can improve infiltrated carbide wear coating systems and 2) to better understand the densification and metallurgical bonding within HDI/TLC coatings. A basic understanding of the dilutive mixing of coating with base material is key to successful technology development. In the proposed work, both applied and fundamental investigations will be conducted. The applied work would develop practical HDI/TLC systems that would be capable of fusing carbide coatings for industrial applications.
Engineering development would focus on developing the process and equipment technology necessary to implement industrial HDI systems that can fuse coatings on such parts. The fundamental research would be aimed at understanding the effect of HDI processing on the coating materials and the subsequent coating properties. This work would develop the necessary materials and process knowledge to enable the control of the HDI process and the proper specification of coating precursor.

Keywords: High Density Infrared Heating Technology, Coatings, Bonding, Corrosion Resistance

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

159. **MATERIALS DEVELOPMENT FOR THE FOREST PRODUCTS INDUSTRY**
$400,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: Peter Angelini (865) 574-4565

The purpose of this project is to determine the cause of failure of composite tubes used in Kraft Black Liquor recovery boilers during pulp and paper making, and to develop new materials to eliminate failures. The project consists of three efforts: 1) to obtain operating data and failure analyses, 2) determination of residual stresses in new and used composite tubes and microstructural characteristics of tubes, and 3) development of new materials and/or fabrication methods for improvements in boiler efficiency, service life, and safety. In FY 2001, the main effort was related to the materials behavior of wall tubes specifically near airports of Kraft recovery boilers. Various companies continued installation of retrofitted parts of floors with the new materials. Temperature measurements of tubes at air ports were continued and results highlighted the influence and significance of thermal cycling on the corrosion/cracking behavior of tubes at those locations. Participants include Oak Ridge National Laboratory (ORNL), Institute of Paper Science and Technology (IPST), the Pulp and Paper Research Institute of Canada (PAPRICAN), 18 pulp and paper companies, and six boiler and materials suppliers.

Keywords: Corrosion, Recovery Boilers, Composite Tubes, Pulp and Paper, Alloys, Stresses, Neutron Residual Stress, Measurements, Modeling, Mechanical Properties

160. **METALS PROCESSING LABORATORY USERS (MPLUS) FACILITY**
$1,000,000
DOE Contact: Mike Soboroff (202) 586-4936
Oak Ridge National Laboratory Contact:
P. Angelini (865) 574-4565

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

161. **DEVELOPMENT OF COMBINATORIAL METHODS FOR ALLOY DESIGN AND OPTIMIZATION**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

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.

Keywords: Combinatorial, Alloys, Casting, Carburization, Corrosion

162. **STOCHASTIC MULTI-OBJECTIVE OPTIMIZATION OF HEAT AND CORROSION RESISTANT ALLOY PROPERTIES**
$186,617
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The project will create a computational modeling tool to customize H-series alloys for specified applications and required properties. The tool will reduce or minimize the need for the addition of expensive alloying elements (including Cr, Ni, Co, Nb, Ti, V) while obtaining the optimum properties needed to design the components. This project focuses on the industry-wide need for improving materials-property performance for the applications that they are currently used for and to increase alloy upper-use temperature, thus leading to improved process efficiencies, including chemical and heat-treating processes carried out at higher temperatures than are currently used. The project takes the new approach of using stochastic optimization algorithms for optimizing H-Series steel compositions with a minimum number of experimental measurements of the composition/properties of candidate alloys. The approach has the potential of identifying new compositions that cannot be identified without carrying out hundreds of experiments. Furthermore, the approach has the potential for creating and designing alloys for specific applications, thereby maximizing their utilization at reduced cost.

Keywords: Computational Modeling, Alloys, Stochastic Optimization Algorithms, Heat Treating, Corrosion

163. **FRACTURE TOUGHNESS AND STRENGTH IN A NEW CLASS OF BAINITIC CHROMIUM TUNGSTEN STEELS**
$124,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

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 percent 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 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. Experiments will be performed on the new class of Fe-3Cr-W(V) steels. Specimens will be prepared at ORNL by vacuum arc melting, solidification, hot rolling, austenitizing at 1050˚C, and normalization in argon. Some of specimens will be tempered at 700˚C. Welding will be also performed on the new class of Fe-3Cr-W(V) steels. The University of Pittsburgh will carry out the microstructure characterization by the use of transmission electron microscopy (TEM) and energy-dispersive spectroscopy (EDS), measure the tensile properties and characterize the microstructure of prestrained specimens by TEM, and determine the fracture toughness by performing JIC tests and subsequent atomic force microscope (AFM) analysis of areas near the crack tip.

Keywords: Steel, Fracture Toughness, Welding, Heat Treating, Microstructure Characterization, Alloys

164. **CHARACTERIZATION AND STRUCTURAL MODELING OF MAGNESIA-ALUMINA SPINEL REFRACTORIES**
$300,565
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goal of the project is to characterize key properties of refractory materials to improve thermal efficiencies and management in industrial combustion environments. Physical and mechanical properties (including creep, thermal conductivity, microstructure, and phase composition) will be evaluated for two spinel glass tank crown refractories. This information will then be used to model and validate the long-term reliability of glass tank crowns.

Keywords: Refractories, Thermal Efficiencies, Mechanical Properties, Glass, Modeling

165. **THERMOCHEMICAL MODELS HIGH-TEMPERATURE MATERIALS PROCESSING AND CORROSION**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936
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

166. **VIRTUAL WELD-JOINT DESIGN INTEGRATING ADVANCED MATERIALS AND PROCESSING TECHNOLOGIES**
$250,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

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

167. **STRESS-ASSISTED CORROSION (SAC) IN BOILER TUBES**
$276,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

The goal of this project is to clarify the mechanisms of 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 will be identified to select parameters for each that reduce the frequency and severity of SAC. In addition, risk factors for SAC will be 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

MATERIALS STRUCTURE AND COMPOSITION

168. **DEVELOPMENT OF COST-EFFECTIVE LOW PERMEABILITY CERAMIC AND REFRACTORY COMPONENTS FOR ALUMINUM MELTING AND CASTING**
$300,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: P. Angelini (865) 574-4459

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 of 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.

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

DEVICE OR COMPONENT FABRICATION, BEHAVIOR, OR TESTING

169. **CONTINUOUS FIBER CERAMIC COMPOSITES (CFCC) - INDUSTRIAL TECHNOLOGIES**
$750,000
DOE Contact: Mike Soboroff (202) 586-4936
ORNL Contact: Peter Angelini (865) 574-4565

The Continuous Fiber Ceramic Composites (CFCC) activity operates as a collaborative effort between industry, national laboratories, universities, and the government to develop advanced ceramic composite materials to a point at which industry will assume full risk of further development. Various industry projects were completed. National laboratories, along with universities, continued the development of supporting technologies (e.g., materials design, processing methods, and sensing technologies) and conducting performance-based evaluations.

Keywords: Continuous Fiber Ceramic Composites, Materials Processing

170. **SELECTIVE INORGANIC THIN FILMS**
$250,000
DOE Contact: Mike Soboroff (202) 586-4936
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. The approach is to nucleate and crystallize zeolithic phases from sol-gel derived amorphous coatings, using porous filters and gas membranes as supports for these films. In FY2001, the R&D continued with advancements made in the fabricability of membrane systems.

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

171. **PHYSICAL AND NUMERICAL ANALYSIS OF EXTRUSION PROCESS FOR PRODUCTION OF BIMETALLIC TUBES**
$200,000
DOE Contact: Mike Soboroff (202) 586-4936

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.

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

172. **HIGH PERFORMANCE, OXIDE DISPERSION STRENGTHENED TUBES FOR PRODUCTION OF ETHYLENE**
$204,956
DOE Contact: Mike Soboroff (202) 586-4936

This project seeks to develop higher-temperature, coking-resistant, fabricable 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.

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

SOLAR ENERGY TECHNOLOGY PROGRAM

	FY 2002
SOLAR ENERGY TECHNOLOGY PROGRAM - GRAND TOTAL	$36,178,000
NATIONAL PHOTOVOLTAICS PROGRAM	$36,178,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$22,488,000
Amorphous Silicon for Solar Cells and Polycrystalline Thin-Film Materials for Solar Cells	14,778,000
Film Silicon for Solar Cells	3,500,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	2,950,000
Nanocrystalline Solar Cell Materials	700,000
Organic Solar Cell Materials	560,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$12,151,000
Materials and Device Characterization	5,297,000
Materials Structure and Composition	6,854,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,539,000
Materials Improvement for High-Efficiency Crystalline Silicon Solar Cells	1,139,000
Instrumentation and Facilities	400,000

SOLAR ENERGY TECHNOLOGY PROGRAM

NATIONAL PHOTOVOLTAICS PROGRAM

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 the 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 2002 is expected to be approximately 540 MW, with about 145 MW made in the U.S.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

173. **AMORPHOUS SILICON FOR SOLAR CELLS AND POLYCRYSTALLINE THIN-FILM MATERIALS FOR SOLAR CELLS**
$14,778,000
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 unintended impurities or undesired structure in the deposited films and by poor uniformity of the films over large (4000 cm^2) areas. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition, and sputtering. The long term goal 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 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, and by controlling the uniformity of deposition over large (4000 cm^2) areas. The films are deposited by chemical and physical vapor deposition, electrodeposition, and 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

174. **FILM SILICON FOR SOLAR CELLS**
$3,500,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contact: Ted Ciszek (303) 384-6569, Ken Zweibel (303) 384-6441 and 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

175. **DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS**
$2,950,000
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, 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

176. **NANOCRYSTALLINE SOLAR CELL MATERIALS**
$700,000
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, Biomimetics

177. **ORGANIC SOLAR CELL MATERIALS**
$560,000
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

178. **MATERIALS AND DEVICE CHARACTERIZATION**
$5,297,000
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, 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, 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

179. **MATERIALS STRUCTURE AND COMPOSITION**
$6,854,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Alex Zunger (303) 384-6672 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

180. **MATERIALS IMPROVEMENT FOR HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS**
$1,139,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Ted Ciszek (303) 384-6569, John Benner (303) 384-6496, and Ed Witt (303) 384-6402

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) and single-crystal silicon made by the Tri-Crystal 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, Tri-Crystals, Heat Exchange Method (HEM)

181. **INSTRUMENTATION AND FACILITIES**
$400,000
DOE Contact: Jeffrey Mazer (202) 586-2455
NREL Contacts: Larry Kazmerski (303) 384-6600 and Pete Sheldon (303) 384-6533

This project procures modern in-house equipment at NREL, primarily for the measurement and characterization of photovoltaic semiconductor materials. This includes equipment for such measurements as ellipsometry, Auger analysis, current-voltage characteristic, Fourier transform-based spectroscopy, electron microscopy; and also includes equipment such as MBE, ECR plasma, and sputtering systems for the fabrication of photovoltaic and related materials.

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

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM

	FY 2002
WEATHERIZATION & INTERGOVERNMENTAL PROGRAM - GRAND TOTAL	$4,777,020
FINANCIAL ASSISTANCE PROGRAM	$4,777,020
INVENTIONS & INNOVATION (I&I)	$2,175,382
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$575,779
A Ceramic Composite for Metal Casting	0
Titanium Matrix Composite Tooling Material for Enhanced Manufacture of Aluminum Die Castings	0
A New Energy Saving Method of Manufacturing Ceramic Products from Waste Glass	0
Energy-Efficient Production and Utilization of Lightweight Structural Panels	0
High Purity Fused Silica Glasses	0
Batch Preheat for Glass and Related Furnace Processing Operations	0
New Membrane Process for Improved Energy Saving Separations in the Petroleum Industry	0
Lost Foam Casting Quantifier Program	46,058
Energy Conservation Waste Reduction in the Processing of Soft (Unfired) Ceramic Particles via Dynamic Cyclone Classification	93,840
Selective Batching for Improved Commercial Glass Melting	40,000
New “Direct Pour In-Mold” (DPI) Technology for Producing Ductile and Compacted Graphite Iron Castings	195,881
Clean Production of Coke from Carbonaceous Fines	200,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$350,134
Development of Phosphors for Use in High-Efficiency Lighting and Displays	0
Energy Saving Lightweight Refractory	0
High Intensity Silicon Vertical Multi-Junction Solar Cells	0
A Low Energy Alternative to commercial Silica-Based Glass Fibers	0
A Viable Inert Cathode for Smelting Primary Aluminum	0
Development of Inert Anode for the Primary Aluminum Industry	0
Automatic Evaluation of Wood Properties	0
Electrochromic Window Film	0
High Throughput Vacuum Processing for Innovative Uses of Glass	123,058
An Insoluble Titanium-Lead Anode for Sulfate Electrolytes	0
Non-Invasive Estimation of Dissolved Alumina Concentration in Hall-Héroult Reduction Cells	29,200
Visible Spectrum Incandescent Selective Emitter	197,876

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM (continued)

	FY 2002
FINANCIAL ASSISTANCE PROGRAM (continued)	
INVENTIONS & INNOVATION (I&I) (continued)	
MATERIALS STRUCTURE AND COMPOSITION	$195,881
Lightweight and Cost Effective Cast Aluminum Diesel Engine Head with Localized Reinforcement	195,881
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$278,105
Fabrication and Testing of a Prototype Ceramic Furnace Coil	0
Fluted Spiral Membrane Module for Reverse Osmosis of Liquids with Dissolved and Suspended Solids	0
High Energy-Density Double-Layer Capacitor Energy Storage for Photovoltaic Systems	158,166
Enabling Tool for Innovative Glass Applications	119,939
INSTRUMENTATION AND FACILITIES	$775,483
Development of an Innovative Energy Efficient High Temperature Natural Gas Fired Furnace	0
Improved Process Control of Wood Waste Fired Boilers	0
Development of Environmentally Benign Mineral Flotation Collectors	0
Thermophotovoltaic Electric Power Generation Using Exhaust Heat in the Glass, Steel and Metal-casting Industries	0
A Hot Eye™ Based Coordinate Measuring Machine for the Forging Industry	69,744
Development of a High-Frequency Eddy-Current Separator	72,058
Integrated Acoustic Kiln Monitor to Guide Accelerated Drying of Wood	108,058
System for Detection and Control of Deposition in Kraft Recovery Boilers and Monitoring Glass Furnaces	113,058
Development and Commercialization of Biopulping	25,058
Development of a Lower pH Copper Flotation Reagent System	108,308
Monitoring of Refractory Wall Recession Using Radar Techniques	40,000
Monitoring of Refractory Wall Recession Using High Temperature Impact-Echo Instrumentation	39,939
Fiber Sizing Sensor/Controller for Optimizing Glass and Polymer Fiber Manufacturing Processes	199,260
NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT AND ECONOMICS (NICE^3)	$2,601,638
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,129,000
Pressurized Ozone Membrane Ultrafiltration Methodology for TDS Removal in Paper Mill Process Water for Energy Savings, Production Efficiency, and Environmental Benefits	0
New Efficient and Safe Direct Hydrogen Peroxide Process	390,000
Energy-savings Regeneration of Hydrochloric Acid Pickling Liquor	0
Demonstration of Magnetic Elutriation Technology for Clean and Efficient Processing Iron Ore	0
Commercial Scale Demonstration of Biopulping: a New Energy-Efficient & Environmentally Benign Technology for Papermaking	468,000

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM (continued)

	FY 2002
NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENTAL AND ECONOMICS (NICE[3]) (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
Catalytic Cracking Demonstration Plant	0
Production-Scale Commercial Demonstration of a Vanadium Carbide Coating Process for Enhancing Wear Resistance of Metals in Steel and Other Manufacturing Industries	0
The Flex-Microturbine for Pecan Waste: Electricity and Heat in a Nutshell	0
Ultra Fine Mineral Recovery Pilot Plant	271,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$738,638
Increased Productivity and Reduced Energy Consumption in Metal-casting Using Titanium Matrix Composite Tooling	395,638
Coated Recouperator	0
Rapid Heat Treatment of Cast Aluminum Components	0
Hot Mill Transfer Bar Edge	0
Clean, Efficient Glass Production Using High Luminosity Oxy-gas Burners	343,000
Plastic Manufacturing from Recovered Post-Consumer Durable Goods	0
MATERIALS STRUCTURE AND COMPOSITION	$0
Lightweight Steel Containers	0
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$234,000
Die Casting Copper Motor Rotors	0
Improvement of the Lost Foam Casting Process	0
Microsmooth Process on Aluminum Wheels	0
Enhanced Application Control of Die Casting Lubricants	0
Commercial Demonstration of an Improved Magnesium Thixomolding Process	0
Zero Emission Mechanical Seal with Integral Micro Heat Exchanger	234,000
Demonstration of a Three-Phase Rotary Separator Turbine	0
Demonstration of a Dual Pressure Euler Steam Turbine for Industrial and Building Applications	0
Adjustable Speed Drives for 500 to 1500 H.P. Industrial Applications	0
INSTRUMENTATION AND FACILITIES	$500,000
Energy Conserving Tool for Combustion Dependent Industries	0
An Automatic High Temperature Steel Inspection and Advice System	500,000
Support Inspection: A Method of Inspecting On-Stream Process Piping at Support Areas	0

WEATHERIZATION & INTERGOVERNMENTAL PROGRAM

FINANCIAL ASSISTANCE PROGRAM

The goal of the Financial Assistance Program of the Office of Weatherization and Intergovernmental Program (OWIP) is to support technologies within the areas of EERE's eleven programs: Solar, Wind & Hydropower, Geothermal, Distribution of Energy & Electrical Reliability, Biomass, Industrial Technologies, FreedomCAR & Vehicle Technologies, Hydrogen, Fuel Cells & Infrastructure, and Building Technologies that have a significant energy savings impact and future commercial market potential. Financial assistance through a competitive solicitation is offered to: 1) speed the development of new energy efficient inventions, and 2) leverage industry and other resources to demonstrate, and promote the benefits of energy savings, pollution prevention and cost savings possible through the adoption of clean, energy-efficient industrial technologies. OWIP provides grants and assistance to independent inventors and small businesses with promising new ideas through its inventions and innovation (I&I) Program. OWIP also provides grants to help fund technology demonstrations through its National Industrial Competitiveness through Energy, Environment and Economics ($NICE^3$) Program. The DOE contact is Lisa Barnett (202) 586-2212

INVENTIONS & INNOVATION (I&I)
DOE Contact: Lisa Barnett (202) 586-2212

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

182. **A CERAMIC COMPOSITE FOR METAL CASTING**
$0
DOE Contact: Keith Bennett (303) 275-4905
MER Corporation Contact: James Withers
(520) 574-1980

The grant will demonstrate nitride/nitride-carbide ceramic composite 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 could be ten times that of coated steel dies.

Keywords: Die Casting, Ceramic Composite, Metal Casting

183. **TITANIUM MATRIX COMPOSITE TOOLING MATERIAL FOR ENHANCED MANUFACTURE OF ALUMINUM DIE CASTINGS**
$0
DOE Contact: Steve Sargent (303) 275-4912
Dynamet Technologies, Inc. Contact:
Susan Abkowitz (781) 272-5967

The grant will produce a metal matrix composite material composed of Ti-6Al-4V and 10-wt percent titanium carbide particulate. The titanium metal matrix composite offers both dramatically improved (400 percent) durability and reduced thermal conductivity (50 percent compared to steel) that will provide energy savings by reducing preheating energy consumption by 4-8 percent.

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

184. **A NEW ENERGY SAVING METHOD OF MANUFACTURING CERAMIC PRODUCTS FROM WASTE GLASS**
$0
DOE Contact: Gibson Asuquo (303) 275-4910
Haun Labs Contact: Michael Haun
(707) 538-0584

The grant will develop a new method to lower energy costs of manufacturing ceramic products. The process calls for the substitution of traditional raw materials with waste glass. Melting temperatures and associated energy consumption will decrease by 35-50 percent by sintering glass powder instead of using traditional ceramic materials.

Keywords: Cullet, Ceramic, Sintering Glass Powder

185. **ENERGY-EFFICIENT PRODUCTION AND UTILIZATION OF LIGHTWEIGHT STRUCTURAL PANELS**
$0
DOE Contact: Gibson Asuquo (303) 275-4910
Genesis Laboratories, Inc. Contact:
Dr. Thomas Owens (630) 879-1112

This grant will demonstrate the feasibility and energy savings of the MWAC method for consolidating and finishing structural cores used in the production of lightweight sandwich panels.

Keywords: Structural Panels, Building Panels, Sandwich Panels

186. **HIGH PURITY FUSED SILICA GLASSES**
$0
DOE Contact: Gibson Asuquo (303) 275-4910
Rensselaer Polytechnic Institute Contact:
Patricia Gray (518) 273-6659

This grant will prepare high purity silica glasses and demonstrate their superior characteristics. High purity silica glasses with superior quality proposed in this work will be supplied to both electronics industry and to optical fiber manufacturers. At the present time, no one holds the technology rights on the proposed method of high purity silica glass production.

Keywords: Glass, Optical Fiber, High Purity Silica

187. **BATCH PREHEAT FOR GLASS AND RELATED FURNACE PROCESSING OPERATIONS**
$0
DOE Contact: Steve Sargent (303) 275-4912
Energy and Environmental Resources Contact:
William Fleming (765) 647-0076

This grant will prepare various salt eutectics in the lab: chlorides of aluminum, iron (III), sodium, calcium, and magnesium will be used in these formulations. The salts will be dissolved in various proportions, and then the water will be evaporated off. Melting points will then be determined in a muffle furnace. The samples which have melting points in the 200-300°F range will then be tested further: in these test, the eutectic salts will be subjected to high temperature exposure (up to 1800°F) in a small lab kiln. The samples will be evaluated thermal stability based on weight loss or evolution of gas/vapor, etc. The eutectic salts will be rated for thermal stability with the top 2 or 3 being tested for corrosivity. The salts will then be used on various metal alloys at up to 1800°F. Finally, corrosivity test will be conducted with metal alloys subjected to sodium sulfate at up to 1800°F.

Keywords: Glass, Glass Furnace, Eutectic Salts, Metal Alloys

188. **NEW MEMBRANE PROCESS FOR IMPROVED ENERGY SAVING SEPARATIONS IN THE PETROLEUM INDUSTRY**
$0
DOE Contact: Doug Hooker (303) 275-4780
(Individual) Contact: Dr. John Dorgan
(303) 277-9033

This grant will demonstrate a new membrane formation process employing a novel solvent and to demonstrate that the membranes produced possess superior properties when compared to existing materials.

Keywords: Petroleum Refining, Membranes, Separations

189. **LOST FOAM CASTING QUANTIFIER PROGRAM**
$46,058
DOE Contact: Steve Sargent (303) 275-4912
Industrial Analytics Corporation Contact:
Pat Alexander (865) 482-8424

This grant will prepare a prototype of a production floor machine and demonstrate it use in a casting improvement program with a major industry partner. Industrial Analytics Corporation is a product and services business engaged in the development and marketing of non-destructive testing and inspection equipment and analysis services for the manufacturing industry. 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 be optimized, production yield can be maximized, quality can be assured, and disputes minimized.

Keywords: Metal Casting, Lost Foam Casting, Non-Destructive Testing

190. **ENERGY CONSERVATION WASTE REDUCTION IN THE PROCESSING OF SOFT (UNFIRED) CERAMIC PARTICLES VIA DYNAMIC CYCLONE CLASSIFICATION**
$93,840
DOE Contact: Steve Sargent (303) 275-4912
InnovaTech, Inc. Contact: Steve Crouch
(919) 881-2197

This grant will confirm prior bench-scale DCC performance through the successful scale-up and testing of a full-sized (2 ton/hr) Beta prototype. A market study and business plan will be produced based on scale-up costs and performance.

Keywords: Ceramics, Dynamic Cyclone Classification, Soft Ceramic Particles

191. **SELECTIVE BATCHING FOR IMPROVED COMMERCIAL GLASS MELTING**
$40,000
DOE Contact: Gibson Asuquo (303) 275-4910
Alfred University Contact: Diane Vossler
(607) 871-2487

This grant will demonstrate that selective pre-batching of raw material feed stocks prior to their introduction to the glass furnace will reduce initial viscosity differences and minimize the tendency for segregation between alkali and alkaline earth salts in the batch. Several binary components will be batched and heated to determine low temperature segregation tendencies. A 10 percent reduction in furnace residence time, resulting in industry-wide savings of 20 trillion Btu/yr. (16 billion cubic feet of natural gas/yr.) is anticipated. A corresponding reduction in energy consumption and CO, CO_2, and NO_x is expected.

Keywords: Glass Melting, Alkali, Alkaline, Earth Salts

192. **NEW "DIRECT POUR IN-MOLD" (DPI) TECHNOLOGY FOR PRODUCING DUCTILE AND COMPACTED GRAPHITE IRON CASTINGS**
$195,881
DOE Contact: Steve Sargent (303) 275-4912
Comanche Technologies Contact:
Jay R. Hitchings (610) 269-6241

This grant will demonstrate and invention combining two proved foundry techniques: in-mold magnesium treatment, and the direct pour method, to produce a unique solution to several problems associated with standard in-mold treatment. It also adds considerable benefits of direct pour. The scope of work is quite broad, combining both the engineering of the container and the marketing work required to understand the optimal launch price as well as best channel(s) to market. DPI containers provide energy savings of 13.3 percent over comparable treatments, increased mold yields, and very high magnesium recovery, zero magnesium fumes, and no post inoculation are required.

Keywords: Pour In Mold, Graphite Iron Casting, Magnesium Treatment

193. **CLEAN PRODUCTION OF COKE FROM CARBONACEOUS FINES**
$200,000
DOE Contact: Doug Hooker (303) 275-4780
Combustion Resources Contact: Craig Eatough
(801) 370-0654

This grant will demonstrate the refine material and process requirements to improve economic benefits and expand prior work on the technology through successful prototype testing of both metallurgical and foundry coke products. The initial market study and business plan will be refined based on this work. A 500,000-ton/year plant that utilizes the new process uses almost six times this amount of waste coke fines as feedstock.

Keywords: Foundry Coke, Carbonaceous Fines, Refine Materials, Metallurgical

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

194. **DEVELOPMENT OF PHOSPHORS FOR USE IN HIGH-EFFICIENCY LIGHTING AND DISPLAYS**
$0
DOE Contact: Andy Trenka (303) 275-4745
Brilliant Technologies, Inc. Contact:
Douglas Kezler (541) 737-6736

This grant will demonstrate and develop 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

195. **ENERGY SAVING LIGHTWEIGHT REFRACTORY**
$0
DOE Contact: Gibson Asuquo (303) 275-4910
Silicon Carbide Products, Inc. Contact:
David Witmer (607) 562-7585

This grant will demonstrate and 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

196. **HIGH INTENSITY SILICON VERTICAL MULTI-JUNCTION SOLAR CELLS**
$0
DOE Contact: Lizana Pierce (303) 275-4727
PhotoVolt, Inc. Contact: Bernard Sater
(440) 234-4081

This grant will demonstrate and develop a low-cost, high-volume fabrication process for high intensity vertical multi-junction (VMJ) solar cells and demonstrate 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.

Keywords: Solar Cells, Solar Concentrators, Photovoltaic

197. **A LOW ENERGY ALTERNATIVE TO COMMERCIAL SILICA-BASED GLASS FIBERS**
$0
DOE Contact: Gibson Asuquo (303) 275-4910
MO-SCI Corporation Contact: Ted Day
(573) 364-2338

This grant will demonstrate and develop 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 400-600o C lower than commercial boro-alumino-silicate glass.

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

198. **A VIABLE INERT CATHODE FOR SMELTING PRIMARY ALUMINUM**
$0
DOE Contact: Keith Bennett (303) 275-4905
PRACSOL, LLC Contact: Robert Rapp
(614) 292-6178

This grant is aimed 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, Cathode, Inert Cathode, Titanium

199. **DEVELOPMENT OF INERT ANODE FOR THE PRIMARY ALUMINUM INDUSTRY**
$0
DOE Contact: Keith Bennett (303) 275-4905
Energy Research Company Contact:
Robert De Saro (718) 442-2725

This grant will experimentally 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 in this project.

Keywords: Aluminum, Anode, Inert Anode, Anode Degradation

200. **AUTOMATIC EVALUATION OF WOOD PROPERTIES**
$0
DOE Contact: Doug Hooker (303) 275-4780
Quantum Magnetics Contact: Erik Magnuson
(858) 566-9200

This grant will determine quantitative, predictive formulas relating wood properties to the solid-state magnetic resonance measurement parameters through the species/class categorization. With the project funds, we will experimentally derive a wood species relationship in terms of magnetic resonance signal parameters, sufficient to allow pallet recyclers to sort wood parts knowing that the reassembled pallets will provide service at least equal to that of a new pallet from similar species material.

Keywords: Pallets, Wood Speciation, Magnetic Resonance, Wood Sorting

201. **ELECTROCHROMIC WINDOW FILM**
$0
DOE Contact: Andy Trenka (303) 275-4745
Chameleon Optics, Inc. Contact: Dr. Paul Martin
(215) 387-2717

This grant will demonstrate manufacturing feasibility of electrochromic window films and to produce samples for further evaluation.

Keywords: Electrochromic Windows, Buildings, Window Film

202. **HIGH THROUGHPUT VACUUM PROCESSING FOR INNOVATIVE USES OF GLASS**
$123,058
DOE Contact: Steve Sargent (303) 275-4912
AVA Technologies, Inc. Contact: Kurt Barth
(970) 491-8411

This grant will demonstrate a system with HPD sources and glass heaters for processing 1 x 1 foot substrates will be developed and tested. A belt arrangement similar that used in the current AVA prototype will be used for transporting substrates from one process module to the next. There will be up to seven processing stations in the vacuum chamber. The processing of complete photovoltaic devices will also be tested.

Keywords: Glass, Photovoltaic Panels, High Pressure Deposition

203. **AN INSOLUBLE TITANIUM-LEAD ANODE FOR SULFATE ELECTROLYTES**
$0
DOE Contact: Steve Sargent (303) 275-4912
Electrodes International Contact: Alla Ferdman (847) 465-0785

The grant will develop 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

204. **NON-INVASIVE ESTIMATION OF DISSOLVED ALUMINA CONCENTRATION IN HALL-HÉROULT REDUCTION CELLS**
$29,200
DOE Contact: Steve Sargent (303) 275-4912
Individual Contact: David Bell (509) 468-0188

This grant will develop a method to identify the dissolved alumina concentration in the Hall-Héroult reduction cell, using estimated properties of the cell resistance disturbance caused by the introduction of suspended alumina particles comprising the normal feed to the cell. The project will optimize this electrochemical process using digital signal processing technology, to assure the process will operate at maximum efficiency. An industry-wide energy improvement of 2 percent current efficiency is expected.

Keywords: Non-Invasive, Alumina, Hall-Héroult, Cells

205. **VISIBLE SPECTRUM INCANDESCENT SELECTIVE EMITTER**
$197,876
DOE Contact: Keith Bennett (303) 275-4905
Sonsight, Inc. Contact: Devon R. McIntosh (301) 283-6250

This grant will design, build, and test a prototype unit of a novel light source that utilizes incandescence with an efficiency and longevity comparable to that of fluorescent lighting. The 18-month project will develop a novel heating arrangement to attain and maintain high, stable incandescent temperatures, and optically and physically optimize the composite ceramic oxide emitter.

Keywords: Incandescent, Emitter, Spectrum, Fluorescent Lighting, Ceramic Oxide

MATERIALS STRUCTURE AND COMPOSITION

206. **LIGHTWEIGHT AND COST EFFECTIVE CAST ALUMINUM DIESEL ENGINE HEAD WITH LOCALIZED REINFORCEMENT**
$195,881
DOE Contact: Steve Sargent (303) 275-4912
Foster-Miller, Inc. Contact: Uday Kashalikar (781) 684-4125

This grant will produce aluminum gravity cast diesel engine head (and block) components for diesel engines with performance and weight comparable to that of current gasoline engines. Highly loaded regions in aluminum gravity castings with metal matrix composites (MMC) will be locally reinforced after being optimized and demonstrated at the subcomponent level.

Keywords: Cast Aluminum, Diesel Engine Head, Localized Reinforcement

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

207. **FABRICATION AND TESTING OF A PROTOTYPE CERAMIC FURNACE COIL**
$0
DOE Contact: Steve Sargent (303) 275-4912
FM Technologies, Inc. Contact: Frederick Mako (703) 961-1051

This grant will 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

208. **FLUTED SPIRAL MEMBRANE MODULE FOR REVERSE OSMOSIS OF LIQUIDS WITH DISSOLVED AND SUSPENDED SOLIDS**
$0
DOE Contact: Doug Hooker (303) 275-4780
Scinsep Systems Contact: Jatal Mannapperuma (530) 758-3708

This grant will develop a methodology for the fabrication of the fluted spiral module, produce a prototype module, and test its performance.

Keywords: Fluted Spiral Membranes, Reverse Osmosis, Separations

209. **HIGH ENERGY-DENSITY DOUBLE-LAYER CAPACITOR ENERGY STORAGE FOR PHOTOVOLTAIC SYSTEMS**
$158,166
DOE Contact: Steve Sargent (303) 275-4912
Heliocentric, LLC Contact: Troy Harvey (801) 427-4748

This grant will scale-up and demonstrate commercial-scale HDLC prototypes, above 1kWh of packaged capacity. Key objectives include further development and improvements in electrode composite, trilaminate composite, the housing, and parameterization of the HDLC variables. HDLC improves energy storage characteristics, reduces embodied energy by 6110 kBtu/kWhC, and lowers photovoltaic system life-cycle cost per kilowatt-hour by 3-5 times. It also improves in-system round-trip energy efficiency by 29-34 percent, and has a 40-60 percent greater available capacity than lead-acid batteries.

Keywords: Capacitor, Energy Storage, Photovoltaic Systems, Batteries

210. **ENABLING TOOL FOR INNOVATIVE GLASS APPLICATIONS**
$119,939
DOE Contact: Gibson Asuquo (303) 275-4910
Michigan Tech. Univ. Contact: Murray Gillis (906) 487-1820

This grant will develop an abrasive waterjet cutting system, using glass as the abrasive media, for new and existing glass production facilities. Objectives include the scaling up and refinement of a circuit used for the production of glass abrasives, the optimization of cutting methods, and utilization of the resulting glass waste stream as filler in various polymers. It is conceivable that a reduction of 10 percent to 15 percent in the size of feedstock will result.

Keywords: Glass, Abrasive Waterjet Cutting, Polymers

INSTRUMENTATION AND FACILITIES

211. **DEVELOPMENT OF AN INNOVATIVE ENERGY EFFICIENT HIGH TEMPERATURE NATURAL GAS FIRED FURNACE**
$0
DOE Contact: Keith Bennett (303) 275-4905
Procedyne Corp. Contact: Vijay Shroff (732) 249-8347

This grant will improve the efficiency of gas-fired furnaces used for heat-treating, metal recovery, and inorganic chemical production. Compared to current gas-fired heating mantles, the proposed furnace can save up to 70 percent of natural gas fuel and achieve a higher combustion efficiency for a given combustion gas discharge temperature.

Keywords: Heat Treating, Gas-Fired Furnaces

212. **IMPROVED PROCESS CONTROL OF WOOD WASTE FIRED BOILERS**
$0
DOE Contact: Jim Spaeth (303) 275-4706
Process Control Solutions Contact: Rick Meeker (850) 385-5100

This grant will characterize the wood-waste boiler control inter-relationships and constraints through data collection and analysis, design an improved control architecture, develop and test an appropriate model predictive control and optimization algorithm, and develop and test a procedure for reproducing the approach and deriving the benefits on all similar pulp and paper wood-waste boilers.

Keywords: Wood-Waste Boiler, Pulp and Paper Boilers, Boiler Architecture

213. **DEVELOPMENT OF ENVIRONMENTALLY BENIGN MINERAL FLOTATION COLLECTORS**
$0
DOE Contact: Steve Sargent (303) 275-4912
Versitech, Inc. Contact: Sharon Young (520) 742-9457

This grant will determine the precise factors that allow the non-sulfur containing triglycerides to collect sulfide minerals, particularly copper, as well or better than the conventional sulfur-containing collectors. The physical and chemical properties of the oils will be measured to try to obtain a correlation between one or more properties or compositions and mineral recoveries. To assist in this effort, artificial oils composed of one type of triglyceride will be tested in order to try to elucidate the best composition for a particular type of ore.

Keywords: Mining, Mineral Flotation, Sulfides, Copper

214. **THERMOPHOTOVOLTAIC ELECTRIC POWER GENERATION USING EXHAUST HEAT IN THE GLASS, STEEL AND METAL-CASTING INDUSTRIES**
$0
DOE Contact: Gibson Asuquo (303) 275-4910
JX Crystals, Inc. Contact: Jason Keyes (425) 392-5237

This grant will build a thermophotovoltaic (TPV) cylinder heated externally with a water-cooled TPV array inside. JX Crystals has developed TPV systems with burners that heat an emitter surrounded by TPV cells. For this project, the heat source is the exhaust stream from an industrial process, so the TPV geometry will be inverted and the circuits will be placed inside an emitter tube. JX Crystals plans to demonstrate the production of 1.5 W/cm^2 of electricity and a TPV efficiency of 20 percent. Additionally, Enron and other companies in the glass, steel and metal casting industries will be contacted in order to familiarize them with TPV and to enlist their support in integrating TPV technology into their processes.

Keywords: Thermophotovoltaic, Photovoltaic, GaSb Cells, Ceramic Emitter

215. **A HOTEYE™ BASED COORDINATE MEASURING MACHINE FOR THE FORGING INDUSTRY**
$69,744
DOE Contact: Steve Sargent (303) 275-4912
OG Technologies Contact: Tzyy-Shuh Chang (734) 769-8500

This grant will develop a 3 dimensional measurement system for the domestic forging industry based on HotEye™. This technology will allow high definition camera to accurately image a red-hot object. The project marries conventional Coordinate Measurement Machine "CMM" technology to HotEye™ technology to permit the accurate measurement of forged parts while they are at high temperature. Being able to take such measurements will dramatically reduce the amount of scrap produced by the domestic forging industry. This industry wastes a significant amount of energy because of the high rate of scrap it produces.

Keywords: Forging, HotEye, Coordinate Measurement

216. **DEVELOPMENT OF A HIGH-FREQUENCY EDDY-CURRENT SEPARATOR**
$72,058
DOE Contact: Steve Sargent (303) 275-4912
EMPS Corporation Contact: Stephen Smoot (801) 582-7600

This grant will confirm prior bench scale testing of the high-frequency eddy-current separator through the successful scale-up and test of a prototype-size unit. The engineering prototype will be demonstrated on contaminated foundry sand at the Eriez test facilities in Erie, PA and on magnesium smut at the Interworld magnesium recovery facility. The initial market study and business plan will be refined based on the results of the prototype unit testing and demonstration.

Keywords: Foundry Sand, Foundries, Separations, Magnesium Smut

217. **INTEGRATED ACOUSTIC KILN MONITOR TO GUIDE ACCELERATED DRYING OF WOOD**
$108,058
DOE Contact: Keith Bennett (303) 275-4905
U.S. Natural Resources Contact: Mark Schafer (610) 832-2100

This grant will complete two pre-production prototypes of the Acoustic Kiln Monitor and demonstrate them in a commercial environment. The ultimate goal is to help operators accelerate lumber drying to its optimal endpoint, while minimizing damage to the wood caused by speeding the drying process.

Keywords: Forest Products, Sensors and Controls, Lumber Drying, Kiln Monitor

218. **SYSTEM FOR DETECTION AND CONTROL OF DEPOSITION IN KRAFT RECOVERY BOILERS AND MONITORING GLASS FURNACES**
$113,058
DOE Contact: Doug Hooker (303) 275-4780
Combustion Specialists Contact: George Kychakoff (425) 432-1589

This grant will finish the development of a system to monitor and control deposition on the pendant tubes of recovery boilers and investigate the applicability of the system to utility boilers and glass furnaces.

Keywords: Forest Products, Kraft Recovery Boilers, Sensors and Controls

219. **DEVELOPMENT AND COMMERCIALIZATION OF BIOPULPING**
$25,058
DOE Contact: Doug Hooker (303) 275-4780
Biopulping International Contact: Masood Akhtar (608) 231-9484

This grant will confirm prior bench-scale testing of the proposed technology through the successful scale-up of the prototype-size in cooperation with a mill.

Keywords: Forest Products, Pulping, Fungus, Wood Chip Penetration

220. **DEVELOPMENT OF A LOWER pH COPPER FLOTATION REAGENT SYSTEM**
$108,308
DOE Contact: Steve Sargent (303) 275-4912
Versitech, Inc. Contact: Sharon Young (520) 742-9457

This grant will develop a system of reagents that can allow mill flotation operators to reduce or eliminate the amount of lime that they use. The system would be pilot plant scale tested to identify and solve any problems that are caused anywhere in the flotation circuit. Possible problem areas include froth bed height in the roughers or the cleaners, recovery losses in the cleaners, and tail flocculation. Froth height problems can be overcome by frother modifications. Loss of recovery in the cleaner can be handled by collector modification, while the flocculation of the tailing can be achieved by changing the flocculent.

Keywords: Mining, Copper, Flotation, Collectors, Flocculation

221. **MONITORING OF REFRACTORY WALL RECESSION USING RADAR TECHNIQUES**
$40,000
DOE Contact: Gibson Asuquo (303) 275-4910
Univ. of Missouri-Rolla Contact: Dr. Robert Moore (573) 341-6326

The project will develop an effective monitoring system that enables glass melters to be managed for optimum efficiency and longevity. The new system will be designed to maximize use and save substantial materials, process energy, and downtime. Research will focus on the recession of refractory walls in contact with commercial glasses and on the adaptation of a special radar technology, the Frequency-Modulated Continuous-Wave Technique, which utilizes simple microwave hardware.

Keywords: Monitoring, Wall Recession, Radar Technology, Glass

222. **MONITORING OF REFRACTORY WALL RECESSION USING HIGH TEMPERATURE IMPACT-ECHO INSTRUMENTATION**
$39,939
DOE Contact: Gibson Asuquo (303) 275-4910
University of Dayton Contact: Claudette Groeber (937) 229-2919

This grant will design and build several high temperature impact-echo transducers to demonstrate their use for measuring the wall thickness of refractory walls used in glass furnaces. Equipment developed will be a pre-prototype system, which may be suitable for industrial trials with only minor refinements.

Keywords: Monitoring, Wall Recession, Impact-Echo Instrumentation, Glass

223. **FIBER SIZING SENSOR/CONTROLLER FOR OPTIMIZING GLASS AND POLYMER FIBER MANUFACTURING PROCESSES**
$199,260
DOE Contact: Gibson Asuquo (303) 275-4910
Powerscope, Inc. Contact: Amir Naqwi (612) 331-4247

This grant will develop a controller for optimizing glass and polymer fiber manufacturing that utilizes real-time, on-line measurements of fiber diameter distribution by laser, used for process monitoring and control. The proposed method uses a collimated laser light beam and an array of ring detectors to collect light diffracted by fibers. Project work involves adaptation of existing technology to fiber sizing and extensive field-testing.

Keywords: Fiber Sensor, Glass Fiber, Polymer Fiber, Laser Light Beam

NATIONAL INDUSTRIAL COMPETITIVENESS THROUGH ENERGY, ENVIRONMENT AND ECONOMICS (NICE^3)
DOE Contact: Lisa Barnett (202) 586-2212

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

224. **PRESSURIZED OZONE MEMBRANE ULTRAFILTRATION METHODOLOGY FOR TDS REMOVAL IN PAPER MILL PROCESS WATER FOR ENERGY SAVINGS, PRODUCTION EFFICIENCY, AND ENVIRONMENTAL BENEFITS**
$0
DOE Contact: David Godfrey (404) 562-0568
Linpac Paper Contact: Joe Gasperetti (864) 463-9090
SC Energy Office Contact: Jean-Paul Gouffray (803) 737-8030

This grant will demonstrate the pressurized ozone membrane ultrafiltration system, from the prototype-sized units, to a production scale commercial demonstration size unit. The project will show that TDS removal can be conducted efficiently and create energy, waste, and economic savings.

Keywords: Total Dissolved Solids, Paper Mill, Pressurized Ozone Membrane Ultrafiltration, Process Water

225. **NEW EFFICIENT AND SAFE DIRECT HYDROGEN PEROXIDE PROCESS**
$390,000
DOE Contact: David Godfrey (404) 347-7140
Princeton Advanced Technology Contact: John Allen (404) 657-7442

This grant will develop a program to build and operate the first commercial unit, where the process can be successfully operated and hydrogen peroxide made for end application testing. The intent is to build a successful commercial demonstration unit to supply customers with hydrogen peroxide.

Keywords: Hydrogen Peroxide, Commercial Hydrogen Peroxide Process

226. **ENERGY-SAVINGS REGENERATION OF HYDROCHLORIC ACID PICKLING LIQUOR**
$0
DOE Contact: Scott Hutchins (617) 565-9765
Green Technology Contact: Doug Olsen (914) 855-0331
CT Bureau of Waste Management Planning & Standards Division Contact: Lynn Stoddard (860) 424-3236

This grant will demonstrate an innovative technology that regenerates spent hydrochloric acid from steel pickling that results in 95 percent energy savings, 52 percent cost savings, and 91 percent reduction in CO_2 over conventional technologies. This process generates no wastewater or residual waste, and produces significant operating and capital cost savings in addition to major energy savings.

Keywords: Hydrochloric Acid Recovery, Pickle Liquor, Galvanizing

227. **DEMONSTRATION OF MAGNETIC ELUTRIATION TECHNOLOGY FOR CLEAN AND EFFICIENT PROCESSING IRON ORE**
$0
DOE Contact: Brian Olsen (312) 353-8579
5R Research Contact: John McGaa (651) 730-4526
MN Dept. Public Service Contact: Jeremy DeFiebre (651) 297-1221

This grant will demonstrate an improved mineral processing technology known as "magnetic elutriation" which increases selectivity when weakly magnetic tailings are separated from magnetic iron ores. This patented process produces yields of 99 percent magnetic iron recovery, while eliminating the need for chemicals used in conventional separation practices. Industry wide, this innovation will reduce chemical use by 1700 tons and save 170 GWh of electrical energy each year.

Keywords: Mining, Magnetic Elutriation, Mineral Processing

228. **COMMERCIAL SCALE DEMONSTRATION OF BIOPULPING: A NEW ENERGY-EFFICIENT & ENVIRONMENTALLY BENIGN TECHNOLOGY FOR PAPERMAKING**
$468,000
DOE Contact: Brian Olsen (312)886-8579
Biopulping International Contact: Masood Akhtar (608) 221-2514
WI Dept. of Administration Contact: Preston Schutt (608) 261-8658

This grant will successfully scale up the technology from the prototype size unit to the production scale commercial size unit and run the commercial demonstration long enough to show successful results and the energy, environmental, and economic benefits. The proposed large-scale trials will be conducted at Andritz, Springfield, Ohio and SENA, Wisconsin Rapids, Wisconsin with final goal of implementing biopulping at the Whiting TMP mill in Wisconsin. Additionally, commercialization activities will continue during the project period to work toward successful commercialization of the technology.

Keywords: Biopulping, Benign Technology, Papermaking, Whiting

229. **CATALYTIC CRACKING DEMONSTRATION PLANT**
$0
DOE Contact: Jack Jenkins (303) 275-4824
Process Innovators Contact: Milton Thacker (801) 943-0241

This grant will demonstrate the Low Profile Fluid Catalytic Cracking Unit (LPFCCU) that improves existing FCCU technology by incorporating the most current technologies and process advances into a low profile multiple reactor unit. The catalyst will be regenerated as in a conventional FCC unit and the products will be fractionated or separated as in a conventional unit.

Keywords: Fluid Catalytic, Cracking Unit, FCU Technology, Low Profile Fluid

230. **PRODUCTION-SCALE COMMERCIAL DEMONSTRATION OF A VANADIUM CARBIDE COATING PROCESS FOR ENHANCING WEAR RESISTANCE OF METALS IN STEEL AND OTHER MANUFACTURING INDUSTRIES**
$0
DOE Contact: Joe Barrett (215) 656-6957
Metlab-Potero Contact: James Coneybear (215) 233-2600
PA Dept. of Environmental Protection Contact: Calvin Kirby (717) 783-9981

This grant will design, install, optimize and operate 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

231. **THE FLEX-MICROTURBINE FOR PECAN WASTE: ELECTRICITY AND HEAT IN A NUTSHELL**
$0
DOE Contact Chris Cockrill (816) 873-3299
Flex Energy Co. Contact: Edan Prabhu (949) 380-4899
AZ Dept. of Environmental Quality Contact: Kathy Charney (602) 207-2254

This grant will demonstrate that the Flex-Microturbine will run on pecan shells, that the Flex-Microturbine can consume this residue cost-effectively and cleanly displacing expensive electricity, and the waste heat is capable of drying and pasteurizing the nuts.

Keywords: Micro-Turbine, Low Btu Gas, Pecan Shells, Nut Orchard Processing

232. **ULTRA FINE MINERAL RECOVERY PILOT PLANT**
$271,000
DOE Contact: Chris Cockrill (816) 873-3299
Graphic Engineering Contact: Ralph Wostenberg (530) 459-5534
CA Energy Commission Contact: Dennis Fukumoto (916) 653-6222

This grant will demonstrate the use of Ultra Fine Mineral Recovery System (UHF) to assure current throughput capacity while at the same time recovering a much higher percentage of minus fifty-micron particles.

Keywords: Mineral Recovery, Fine Minerals, UHF

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

233. **INCREASED PRODUCTIVITY AND REDUCED ENERGY CONSUMPTION IN METAL-CASTING USING TITANIUM MATRIX COMPOSITE TOOLING**
$395,638
DOE Contact: Scott Hutchins (617) 565-9765
Dynamet Technology Contact: Susan M. Abkowitz (781) 272-5967

This grant will demonstration that titanium matrix composite tooling materials can be used in the die casting industry as a liner for shot sleeves By these demonstrations energy, environmental and economic data will be accumulated to substantiate or to modify the expectations for this technology. By the end of this program, the CermeTi liners and possibly related components will be ready for commercialization in the industry. The data and experience gained will be used to encourage wide spread commercial use.

Keywords: Die Casting, Shot Sleeves, Titanium Matrix, Metal-Casting, Composite Tooling

234. **COATED RECOUPERATOR**
$0
DOE Contact: Brian Olsen (312) 886-8579
Alcoa Contact: David Williams (724) 337-2861
IN Dept. of Commerce Contact: Niles M. Parker (317) 232-8939

This grant will demonstrate the full-scale use of a corrosive-resistant coating that extends the operational life of recuperators used in aluminum melting furnaces. Objectives include achieving a recuperator life of four years or more, allow for use of less expensive HL material, and show that a coated standard metallic recuperator costing $125,000 will last for four years or more. Operation of a standard Alcoa aluminum furnace with the novel coating is expected to bring annual energy savings of 5 trillion Btu, a waste reduction of 3,517 tons, and cost savings of $46,147.

Keywords: Recouperator, Corrosive-Resistant Coating, Aluminum Melting Furnace

235. **RAPID HEAT TREATMENT OF CAST ALUMINUM COMPONENTS**
$0
DOE Contact: Brian Olsen (312) 886-8579
Technomics Contact: Steve Krause (612) 475-1752
MN Dept. Public Service Contact: Jeremy DeFiebre (651) 297-1221

This grant will design, build, and operate a full-scale facility for demonstrating to manufacturers, with their own cast aluminum components, a novel automated in-line heat-treating and quenching system. This system uses fluidized bed technology that reduces the time required to achieve specifications by 80-90 percent. The system is expected to cut energy use by 90 percent.

Key words: Heat Treatment, Cast Aluminum, Automated In-Line Heat Treatment

236. **HOT MILL TRANSFER BAR EDGE**
$0
DOE Contact: Joe Barrett (215) 656-6957
Weirton Steel Contact: Frank Tluchowski (304) 797-2296

This grant will produce higher quality steel having less edge related defects using less natural gas and proportionally reducing CO_2 and NO_x emissions at the furnaces. The oxy-gas burners and associated accessories developed by Air Products and Chemicals, Inc. in conjunction with Daniell-United will be installed at Weirton Steel to demonstrate the technology. Based on a plant producing 3 million tons of steel coil annually, natural gas consumption will be decreased by 28 percent, CO_2 emission will be cut by 1,310 tons, and strength and ductility of the final product is increased compared to conventional heating.

Keywords: Hot Mill, Oxy-Gas Burners, Bar Edge

237. **CLEAN, EFFICIENT GLASS PRODUCTION USING HIGH LUMINOSITY OXY-GAS BURNERS**
$343,000
DOE Contact: Joe Barrett (215) 656-6957
PPG Industries Contact: Robert P. Woelke (412) 820-8142
PA Dept. of Environmental Protection Contact: Calvin Kirby (717) 783-9981

This grant will scale up and demonstrate the High Luminosity burner with integrated combustion actuators and controllers as the permanent combustion system for an oxy gas fired flat glass furnace and to achieve significant decreases in energy consumption, improvements in furnace operation, and decreases in gaseous emissions.

Keywords: Glass Production, Oxy-Gas Burners, High Luminosity

238. **PLASTIC MANUFACTURING FROM RECOVERED POST-CONSUMER DURABLE GOODS**
$0
DOE Contact: Chris Cockrill (816) 873-3299
MBA Polymer Contact: Laurence Allen (510) 231-9035
NYSERDA Contact: Dana Levy (518) 862-1090

This grant will construct and demonstrate a plant that sorts various plastics or polymers. The technology utilizes a novel differentiation technology that allows density-based sorting of various plastics to occur. Different types of plastics or different grades of the same plastic can now be efficiently sorted to obtain a pure, singular end product.

Keywords: Plastic Manufacturing, Sorting Plastics, Post-Consumer Durable Goods

MATERIALS STRUCTURE AND COMPOSITION

239. **LIGHTWEIGHT STEEL CONTAINERS**
$0
DOE Contact: Joe Barrett (215) 656-6957
Dispensing Container Contact: George Diamond (908) 832-7882

This grant will demonstrate a thin-walled dispensing container as strong as conventional steel containers that utilize an average of 1.7 ounces of steel, or a reduction from conventional containers of approximately 40 percent. Work includes: a) designing bottom shape, b) determining bottom metal thickness and, c) exploring methods of manufacturing the bottom. Additional work to test various pressurizing agents will be done. For a plant producing 200 million containers each year, savings will amount to more than 500 billion Btu for large containers and 200 billion Btu for small containers.

Keywords: Thin-Walled Container, Lightweight Steel, Containers

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

240. **DIE CASTING COPPER MOTOR ROTORS**
$0
DOE Contact: Scott Hutchins (617) 565-9765
ThermoTrex Contact: John McCoy (619) 646-5403

This grant will demonstrate high temperature, thermal shock resistant materials that withstand the copper motor rotor dye-casting environment for an economically acceptable life. A cost effective near-net shape material forming process, named Chemical Vapor Composites, will be utilized. Substantial energy and waste savings are expected.

Keywords: Die Casting, Copper Motor, Motor Rotor, Resistant Materials

241. **IMPROVEMENT OF THE LOST FOAM CASTING PROCESS**
$0
DOE Contact: Scott Hutchins (617) 565-9765
GM Contact: Charles Gough (248) 857-2841
NYSERDA Contact: Dana Levy (518) 862-1090

This grant will evaluate and improve 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

242. **MICROSMOOTH PROCESS ON ALUMINUM WHEELS**
$0
DOE Contact: Scott Hutchins (617) 565-9765
Metal Arts Contact: Stanley Dahle (315) 789-2200
NYSERDA Contact: Dana Levy (518) 862-1090

This grant will demonstrate the use of an innovative electroless nickel-plating process, using the Microsmooth process, a streamlined replacement for conventional process nickel/chrome plating used in aluminum product finishing. Chemistry will be optimized and protocols will be tested to determine the best possible product and system for demonstration. Using Microsmooth is expected to reduce energy and chemical usage, thus providing environmental, economic, and worker health benefits.

Keywords: Microsmooth Process, Aluminum Wheels, Nickel-Plating Process

243. **ENHANCED APPLICATION CONTROL OF DIE CASTING LUBRICANTS**
$0
DOE Contact: Brian Olsen (312) 886-8579
N. Amer. Die Casting Assoc. Contact: Steve Udvardy (847) 292-3600

This grant will utilize a controlled; two-step energy and pollution reducing technique where water is applied to cool die surfaces during die casting operations. The technology will be demonstrated at Spartan Light Metal Products in Sparta, Illinois. 50 percent of lubricant used by the old method can be saved, meaning potential industry-wide reductions of emissions by 1440 tons, and 2880 tons of waste liquid per year. Operation of one die casting machine with the new technology will save 6 billion Btu/year.

Keywords: Application Control, Die Casting, Lubricants, Emissions

244. **COMMERCIAL DEMONSTRATION OF AN IMPROVED MAGNESIUM THIXOMOLDING PROCESS**
$0
DOE Contact: Brian Olsen (312) 886-8579
Thixomat, Inc. Contact: Dr. Ray Decker (734) 995-5550
State of Michigan, Energy Division Contact: John Trieloff (517) 241-6224

This grant will demonstrate 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

245. **ZERO EMISSION MECHANICAL SEAL WITH INTEGRAL MICRO HEAT EXCHANGER**
$234,000
DOE Contact: Jack Jenkins (303) 275-4824
Exxon/Mobil Contact: Karl Simpson (225) 977-1920
LA Dept. of Natural Resources Contact: Paula Ridgeway (225) 342-2133

This grant will demonstrate the attraction of a mechanical seal OEM to the commercialization team (which now consists of LSU, UK and Mezzosystems) by successfully demonstrating the reliability and performance of the mechanical seal at a major end user facility (ExxonMobil). This industrial application with a light hydrocarbon as the process (sealed) fluid will be ideal to demonstrate: 1) heat tolerance; 2) long term reliability; 3) energy impact; 4) environmental impact and 5) economic impact.

Keywords: Zero Emission, Mechanical Seal, Heat Exchanger, Hydrocarbon

246. **DEMONSTRATION OF A THREE-PHASE ROTARY SEPARATOR TURBINE**
$0
DOE Contact: Chris Cockrill (816) 873-3299
Douglas Energy Co. Contact: Lance Hays (714) 524-3338
CA Energy Commission Contact: Dennis Fukumoto (916) 653-6222

This grant will demonstrate a newly developed compact separator for the petroleum industry which utilizes previously wasted process energy to generate power and separate gas, oil, and water. This technology, to be demonstrated at a Chevron 15,000 barrel per day facility, will substantially improve the efficiency and productivity of high-pressure offshore oil and gas drilling operations.

Keywords: Oil and Gas Production, Hydrocarbon Separation, Petroleum

247. **DEMONSTRATION OF A DUAL PRESSURE EULER STEAM TURBINE FOR INDUSTRIAL AND BUILDING APPLICATIONS**
$0
DOE Contact: Chris Cockrill (816) 873-3299
Douglas Energy Contact: Lance Hays (714) 524-3338
CA Energy Commission Contact: Dennis Fukumoto (916) 653-6222

This grant will demonstrate the Euler Dual Pressure Steam Turbine, a unique turbine system that dramatically improves generation efficiency by utilizing energy that was previously wasted by releasing it through the letdown valves of single steam turbine systems. The demonstration unit will be installed at the Rolex Building in New York City where it will replace a standard generating unit and produce more than 200 megawatts of additional electricity. Turbine efficiency is expected to increase to 80 percent, thus doubling what is currently possible.

Keywords: Steam Turbine, Dual Pressure, Generation Efficiency

248. **ADJUSTABLE SPEED DRIVES FOR 500 TO 1500 H.P. INDUSTRIAL APPLICATIONS**
$0
DOE Contact: Chris Cockrill (816) 873-3299
MagnaDrive Contact: Bruce Densmore (206) 336-5717

This grant will scale-up the 1500 horsepower MagnaDrive Adjustable Speed Coupling System (ASCS) from a working prototype to the production-scale commercial ASCS. MagnaDrive will install this innovative, energy efficient speed control technology at four industrial sites where they will be monitored for energy, environmental, and economic benefits. When compared to competing technology, the ASCS will save 20 percent of pump energy and 15 percent of fan energy consumed during continuous operation.

Keywords: Adjustable Speed, Coupling System, Industrial Applications

INSTRUMENTATION AND FACILITIES

249. **ENERGY CONSRVING TOOL FOR COMBUSTION DEPENDENT INDUSTRIES**
$0
DOE Contact: Scott Hutchins (617) 565-9765
AFR Contact: James Markham (860) 528-9806
CT Bureau of Waste Management Planning & Standards Division Contact: Lynn Stoddard (860) 424-3236

This grant will demonstrate a new, portable, low-cost, energy-efficient multi-gas analyzer for industries utilizing combustion boiler and turbine systems. This state-of-the-art combustion-tuning tool saves substantial fuel, reduces emissions, and validates pollution abatement/control technology.

Keywords: Combustion Tuning, Multi-Gas Analyzer, Boiler, Turbine System

250. **AN AUTOMATIC HIGH TEMPERATURE STEEL INSPECTION AND ADVICE SYSTEM**
$500,000
DOE Contact: Brian Olsen (312) 886-8579
OG Technologies Contact: Terence C. Libby (734) 769-8500
IN Dept. of Commerce Contact: Niles M. Parker (317) 232-8939

This grant will design and build a production scale HE SteelerTM system and install it at the exit of the rod mill at Inland Steel's 12" Bar Mill in Indiana. OGT will operate the system for 180 days, collect and analyze the data from the system and work with Inland Steel to determine appropriate process corrections based on the analysis. The objectives will be to demonstrate that the system: 1) operates reliably under actual production conditions; 2) identifies 99 percent of the surface defects present during production; 3) measures the size of the product to within +/1 percent of bar diameter; and 4) reduces the amount of scrap being produced from 5 percent to 2.5 percent.

Keywords: Steel Inspection, Advice System, Rod Mill

251. **SUPPORT INSPECTION: A METHOD OF INSPECTING ON-STREAM PROCESS PIPING AT SUPPORT AREAS**
$0
DOE Contact: Jack Jenkins (303) 275-4805
Tubular Ultrasound Contact: David Siverling (713) 426-1072
Texas Natural Resource Conservation Commission Contact: Jeff Voorhis (512) 239-3178

This grant will demonstrate to the petrochemical industry the first commercial system to quantify the remaining wall thickness of on-stream piping at pipe supports. The first Support Inspection system demonstration will be used for a series of full-scale commercial demonstrations, evaluations, and certifications at world-class domestic petrochemical facilities.

Keywords: Pipe Support Inspection, Petrochemical, Ultrasound

OFFICE OF SCIENCE

	FY 2002
OFFICE OF SCIENCE - GRAND TOTAL	$539,912,655
OFFICE OF BASIC ENERGY SCIENCES	$490,258,000
DIVISION OF MATERIALS SCIENCES AND ENGINEERING	$490,258,000
Theoretical Condensed Matter Physics	18,007,000
Experimental Condensed Matter Physics	33,667,000
Materials Chemistry	27,287,000
Mechanical Behavior and Radiation Effects	14,530,000
X-ray and Neutron Scattering	35,032,000
Structure and Composition of Materials	35,168,000
Physical Behavior	15,735,000
Synthesis and Processing Sciences	14,497,000
Engineering Physics	16,464,000
Experimental Program to Stimulate Competitive Research	7,679,000
X-ray and Neutron Scattering Facilities	268,032,000
Nanoscience Centers	4,160,000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH	$41,254,655
DIVISION OF TECHNOLOGY RESEARCH	$41,254,655
LABORATORY TECHNOLOGY RESEARCH PROGRAM	$1,545,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,020,000
Advanced Processing Techniques for Tailored Nanostructures in Rare-Earth Permanent Magnets (AL 01 02)	198,000
Development of Bismuth-Based Superconducting Wire with Improved Current Carrying and Flux Pinning Properties (ANL 99 15)	96,000
Interplay Between Interfacial and Dielectric and Ferroelectric Behaviors of Barium Strontium Titanate Thin Films (PNL 99 08)	118,000
Advanced Computational Models and Experiments for Deformation of Aluminum Alloys–Prospects for Design (PNL 99 07)	90,000
Near-Frictionless Carbon Coatings (ANL 98 03)	19,000
Interfacial Properties of Electron Beam Cured Composites (ORNL 99 08)	105,000
Photocatalytic Metal Deposition for Nanolithography (ANL 99 13)	205,000
Low-Cost, High-Performance YBCO Conductors (ORNL 01 06)	189,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$525,000
Nanofabrication of Advanced Diamond Tools (LBNL 01 03)	150,000
Development of a High-Efficiency Rotary Magnetocaloric Refrigerator Prototype (AL 99 02)	125,000
Direct Casting of Titanium Alloy Wire for Low-Cost Aerospace and Automotive Fasteners (PNL 99 02)	73,000
Nonconsumable Metal Anodes for Primary Magnesium Production (ANL 98 05)	110,000
Optimized Catalysts for the Cracking of Heavier Petroleum Feedstocks (LBNL 99 01)	67,000

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS INNOVATION RESEARCH PROGRAM	$37,722,980
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$17,445,526
PHASE I	$4,174,621
Silicon Carbide High Temperature Dynamic Pressure Gauge	99,632
Turbine Blade Emissivity Sensor	100,000
Development of Robust NO_x Monitor	98,856
Amorphous, Non-Oxide Seals, Derived from Organic Precursors, for Solid Oxide Fuel Cells	97,026
Perovskite/Oxide Composites as Mixed Protonic/Electronic Conductors for Hydrogen Recovery in IGCC Systems	99,980
Highly Textured Composite Seals for SOFC Applications	100,000
Internal Pipe Repair System	99,929
Assure Natural Gas and Oil Pipeline Reliability by Cost-Effective, High-Performance Thermoplastic Liners	98,802
Biomimetic Membrane for Carbon Dioxide Capture from Flue Gas	99,842
Catalysts and Membrane for Selective Methane Oxidative Dimerization	100,000
High Efficiency Amorphous and Microcrystalline Silicon Based Double-Junction Solar Cells Made with Very-High-Frequency Glow Discharge	100,000
Low-Cost Nanoporous Sol Gel Separators for Lithium-Based Batteries	100,000
The Development of a Low-Cost Separator with Improved Performance	99,969
New Solid State Lighting Materials	99,957
Monomer-Excimer Phosphorescent White OLEDS for General Lighting	100,000
White Illumination Sources Using Striped Phosphorescent OLEDs	100,000
An Approach for Reducing Wind Turbine Tower Weight by 70 Percent by Combining an Innovative On-Site Manufacturing Method with a Novel Tower Design	99,702
Development of a Low Wind Turbine Blade Making Optimal Use of Carbon Fiber Composites	99,968
Utilization of Isotruss Technology in Taller Wind Turbine Towers	100,000
Transformer Ratio Enhancement Experiment for Next Generation Dielectric Wakefield Accelerators	90,300
Inexpensive High Quality Electron Sources	100,000
Continuous Formation of Ta Barrier and Cu Sheath of Nb_3Sn Subelements	100,000
Concentric Tilted Double-Helix Dipole Magnets	99,976
Multifilament Extrusion Cuprate Superconductors	92,953
Advanced, High-Filament-Count, Nb_3Al, Jelly-Roll Strand for Accelerator Applications	100,000
Eliminating a Major Cause of Wire Drawing Breakage in A-15 High-Field Superconductors	100,000
Optimization and Commercialization of the Cable-In-Tube Approach to Fabricating High Performance Nb_3Sn Wires	100,000
High Current Density (Jc), Low AC Loss, Low Cost Internal-Tin Superconductors	99,968
Hybrid Electrochemical - Electrolytic Capacitor for Next-Generation Electron-Positron Linear Collider	99,977
Microwave Component Fabrication using the Fast Combustion Driven Compaction Process	99,784
A High Thermal Performance, Self-Contained Heat Extraction System suited to Highly Distributed Heat Sources, with Premise Based on Ultra-Lightweight Considerations	99,797
Cylindrical Electrode-Less Gas Electron Multiplier	99,324
Micro-Photomultiplier Array	100,000
Electrically Medicated Microetching Manufacturing Process to Replace Emersion and Spray Etching	99,859
Radiation Hard Lead Zirconium Titanium (PZT) for Ferroelectric and Plezoelectric Devices	99,920

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
PHASE I (continued)	
Innovative Helium-Cooled Tungsten PFCs	100,000
Insulators and Materials for Close-Spaced Thermoelectric Modules	99,999
Separation and Enrichment of Xenon in Air	100,000
A Small Seismic Accelerometer Utilizing Single Crystal Piezoelectric Material	99,591
High Performance Thermo-Electrically-Cooled LWIR Mercury Cadmium Telluride Detectors	100,000
Nano Liter Scale Blood Sampling and Analysis System	100,000
VEGF-Based Delivery of Boron Therapeutics	99,510
PHASE II (FIRST 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
Amened 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
PHASE II (SECOND YEAR)	$8,459,941
Non-Linear Optical Devices for High Performance Networking, Computing and Telecommunication Routing and Modulating	375,000
Advanced Geothermal Optical Transducer (AGOT)	325,879
Fast-Response, Two-Dimensional Detector for Epithermal Neutron Detection with Adjustable Shape	374,999
Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors	300,000
Affinity Ceramic Membranes with Carbon Dioxide Transport Channel	300,095
Photocatalytic Membranes for Producing Ultrapure Water	300,000
Novel Membrane Reactor for Fischer-Tropsch Synthesis	300,000
Fast, Low-Noise Readout Chip for Avalanche Photodiode Arrays for Use in Positron-Emission Tomography Imaging	340,000
Miniature Electrochemical Carbon Dioxide Detector	338,128
An Innovative Ultramicroelectrode Array for Field-Deployable Trace Metal Analysis	340,000
Novel Joining Technique for Oxide-Dispersion Strengthened Iron Aluminide Alloys	375,000
A Metallic Interconnect for Intermediate Temperature, Planar, Solid Oxide Fuel Cells	325,000
Tailorable, Inexpensive Carbon Foam Electrodes for High-Efficiency Fuel Cell and Electrochemical Applications	375,000
Advanced Cathode Structure for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cells	350,000

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
PHASE II (SECOND YEAR) (continued)	
Efficient Incandescent Lighting Based on Selective Thermal Emitters	350,000
‘On Chip' Smart Sensor Array and Control Teleplatform for Thermophotovoltaic Cell Manufacturing Applications	350,000
Infrared Focal Plane Array with Fast Shuttering	375,000
Linear Avalanche Photodiode Detector Arrays for Gated Spectroscopy with Single Photon Sensitivity	375,000
Development of a Large-Area Mercuric Iodide Photodetector for Scintillation Spectroscopy	374,285
Segmented, Deep-Sensitive-Depth Silicon Radiation Detectors	366,561
Micromachined Silicon, Large Area X-Ray Detector	374,994
Cost-Reduction Techniques for Powder-in-Tube Niobium-Tin Superconductors	300,000
Flexible Niobium-Tin Cables Suitable to React-then-Wind Approach to Fabricating Accelerator Magnets	250,000
Novel Avalanche Photodiode Arrays for Scintillating Fiber Readout	375,000
Manufacturing of Robust Ceramic/Metal Joints for Alkali Metal Thermalto Electric Converters	250,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$4,167,368
PHASE I	$797,701
Multilayer Composite Membranes for Upgrading Acid-Rich Natural Gas	100,000
Low-Temperature, Solid Oxide Fuel Cell Cathode Development	99,694
Use of Graphite Nanofibers as a Catalyst for the Synthesis of Styrene	100,000
Modeling of Copper-Indium-Gallium Diselenide for Advanced Thin-Film Photovoltaic Devices	100,000
Stabilized Lithium Manganese Oxide Spinel Cathode for High Power Li-Ion Batteries	98,055
A Multi-Megawatt Continuous Wave RF Window for Particle Accelerator Applications	100,000
An IR Imaging and Spectral Diagnostic System for Alcator C-Mod	99,952
A Solid-State Irradiance Calibrator for Field Use	100,000
PHASE II (FIRST 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

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
PHASE II (SECOND YEAR)	$700,000
Utilization of Hydrocarbon Fuels in Low-Temperature Solid Oxide Fuel Cells	375,000
Thin Alternatives to Braided Glass Insulation for Low-Temperature Superconducting Wire	325,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$13,783,998
PHASE I	$4,298,911
Embedded Sensors in Turbine Systems by Direct Write Thermal Spray Technology	99,769
Contamination Resistant Anodes for Intermediate Temperature Solid Oxide Fuel Cells	99,998
CU-SDC Nanostructural Electrodes as Coking-Resistant Anodes for intermediate-Temperature SOFCS	100,000
Low-Cost Protective Layer Coatings on Thermal Barrier Coatings via CCVD	100,000
A Commercially Viable Carbon Molecular Sieve Membrane for Subquality Natural Gas	100,000
Catalyst to Improve Small-Scale Claus Plants	100,000
LSGM Based Composite Cathodes for Anode Supported, Intermediate Temperature (600-800 degrees C) Solid Oxide Fuel Cells (SOFC)	99,953
Advanced Structural Carbon-Supported Catalysts for Industrial Polymer Synthesis	99,999
Metal Oxide Catalyst for Methacrylic Acid Preparation via One-Step Oxidation of Isobutane	99,988
Solid-Acid Catalyst for Refinery Alkylation	100,000
Structured Catalyst for Exothermic Reactions	100,000
Development of Ion Beam Techniques for Layer Splitting of Oxide Materials	99,982
A Novel Technique to Produce Ultra-Porous Metallic Foams through Thermal Reduction of Nano-Particle Oxide	100,000
Novel High Temperature Polymer Substrate for Low Cost High Efficiency Thin Film CIGS Solar Cells	99,728
Non-Vacuum Techniques for Front and Back Contacts for CIGS Solar Cells	99,795
Transparent Conducting Oxide Films with High Refractive Index	100,000
P-Type ZnO Films	100,000
An Advanced Cathode Material for Li-Ion Battteries	100,000
Polymer and Gel Electrolyte for Lithium Sulfur Batteries	100,000
The Development of a Polyvalent Battery System	99,965
Synthesis & Integration of Quantum Confined Atom (QCA) Nanophosphor Based Down Converter for AlInGaN-Based High Luminous Efficiency White-Light LED Lamps	99,933
General Illumination Using Dye-Doped Polymer Light Emitting Devices	99,998
Nanomaterials-Based Electrodes for High Charge Rate Energy Storage Devices of HEVs	100,000
Supported Urania Catalysts for Fatty Acid Methyl Ester Dehydrogenation	100,000
Three-Dimension Woven Carbon-Glass Hybrid Wind Turbine Blades	100,000
PIT Nb_3Sn Superconducting Strands Based on a Modified Powder/Tube Reaction Route	100,000
Non-Copper Jc of 2800 A/mm^2 through Optimization of PIT Nb_3Sn Conductor Design	100,000
An Elemental Powder Approach for High Performance Nb_3Sn Superconductors	100,000
Feasibility of Cost Effective, Long Length, BSCCO 2212 Round Wires, for Very High Field Magnets, Beyond 12 Tesla at 4.2 Kelvin	100,000
A New Method for Depositing Niobium Films for Niobium/Copper Cavities	100,000
Growth of a New, Fast Scintillator Crystal for Nuclear Experiments	99,997

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
PHASE I (continued)	
A Superior Scintillator Material for High Resolution X-Ray Detectors	100,000
A New Scintillator for Gamma Ray Spectroscopy	100,000
Diamond Windows for High Power Microwave Transmission	100,000
Radiation Resistant Insulation with Improved Shear Strength for Fusion Magnets	100,000
Nanostructured Tungsten for Improved Plasma Facing Component Performance	100,000
High-Strength, High-Conductivity Composite for Plasma Facing Applications	100,000
Rugged Packaging for Damage Resistant Inertial Fusion Energy Optics	99,922
Low Cost Materials for Neutron Absorption in Generation IV Nuclear Power Systems	99,960
High Resolution Gamma Ray Spectrometer for Nuclear Non-Proliferation	100,000
Growth of a New Mid-IR Laser Crystal	99,964
Ultrapurification, Crystal Growth, and Characterization of Rare-Earth Doped KPb_2Br_5 for Mid-Infared Lasers	100,000
Induim Arsenide Antimonide Very Long Wavelength Photodiodes for Near Room Temperature Operation	99,960
PHASE II (FIRST 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 MesoCarbon 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
PHASE II (SECOND YEAR)	$3,922,654
The Development and Demonstration of Reliable Adherent Metalization of AIN	375,000
Novel Lithium-Ion Conducting Polymer Electrolytes for Lithium-Ion Batteries	374,997
Synthesis of New Solid Polymer Electrolytes	374,999
Membranes for Reverse Organic-Air Separations	300,000
Hydrogen Recovery Process Using New Membrane Materials	300,000
New Boronated Amino Acids for Neutron Capture Therapy	268,028
Low-Cost Arc Process to Produce Single-Walled Nano-Tubes Using Coal-Based Starting Materials	300,000
Novel Catalyst for Carbon Monoxide Removal from Fuel Cell Reformate	355,000
A Fast, High Light Output Scintillator for Gamma Ray and Neutron Detection	375,000

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
PHASE II (SECOND YEAR) (continued)	
In-Situ Electron Beam Processing for Radio Frequency Cavities	300,000
An Innovative Fabrication Concept for Niobium-Tin Superconducting Wire	299,630
High-Performance Niobium-Tin-Tantalum Superconductors Formed by Mechanical Alloying and Near-Net Shape Tube Filling	300,000
INSTRUMENTATION AND FACILITIES	$2,126,252
PHASE I	$628,138
An Inexpensive, Efficient Neutron Monochromator	100,000
High Performance Thermal Neutron Detector	100,000
Neutron and Electron Beam Instrumentation (MSC P1A20-205)	99,802
High Gain, Fast Scan, Broad Spectrum, Parallel Beam Wavelength Dispersive X-ray Spectrometer for SEM	60,023
Advanced X-ray Detectors for Transmission Electron Microscopy	100,000
Using Convergent Beams for Small-Sample, Time-of-Flight Neutron Diffraction	98,713
Four Probe Stage and Holder for Transmission Electron Microscope	69,600
PHASE II (FIRST 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	$199,836
PHASE I	
LITS-Forming for Pre-Bending of Alumiunum Hydroformed Truck Frames	99,858
Development of a New, Low Frequency, Rf-Focused Linac Structure	99,978
SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM	$1,986,675
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$550,000
PHASE I	$300,000
Carbon Fiber Composite Aeroelastically Tailored Rotor Blades for Utility-Scale Wind Turbines	100,000
Insulation Coating of Rutherford Cable for Accelerator Applications	100,000
Fiber Optic Scintillator System for Detection of Beta Emitters in Groundwater	100,000

OFFICE OF SCIENCE (continued)

	FY 2002
SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
PHASE II (FIRST YEAR)	$250,000
Advanced Membrane Technology for Biosolvents	250,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$450,000
PHASE I	$200,000
Hydroforming of Light Weight Components from Aluminum and Magnesium Sheet and Tube	100,000
Carbon/Glass Hybrid Wind Turbine Blades	100,000
PHASE II (FIRST YEAR)	$250,000
Neutron Scattering Instrumentation for Measurement of Melt Structure	250,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$986,675
PHASE I	$100,000
Waveshifters and Scintillators for Ionizing Radiation Detection	100,000
PHASE II (FIRST 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 FUSION ENERGY SCIENCES	$8,400,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,400,000
Vanadium Alloy and Insulating Coating Research	2,000,000
Theory and Modeling	1,200,000
Ferritic/Martensitic Steel Research	1,900,000
SiC/SiC Composites Research	1,500,000
Plasma Facing Materials Research	1,800,000

OFFICE OF SCIENCE

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 Advanced Scientific Computing Research - Division of Advanced Energy Projects and 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 are available on the World Wide Web at the following address: http://www.sc.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 2002 funding for this program is $18,007,000 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 2002 funding for this program is $33,667,000 and the DOE contact is Dale D. Koelling, (301) 903-2187.

MATERIALS CHEMISTRY

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 2002 funding for this program is $27,287,000 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 defect-behavior 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 non-crystalline 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 2002 funding for this program is $14,530,000 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 2002 funding for this program is $35,032,000 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 2002 funding for this program is $35,168,000 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 2002 funding for this program is $15,735,000 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 2002 funding for this program is $14,497,000 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 2002 funding for this program is $16,464,000 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 2002 funding for this program is $7,679,000 and the DOE contact is Matesh Varma, (301) 903-3209.

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 next-generation 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 X-ray light source. The FY 2002 funding for this program is $268,032,000 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. Nano-science 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 nano-fabrication with advanced tools for nano characterization. The NSRCs will become a cornerstone of the Nation's nanotechnology revolution, covering the full spectrum of nano-materials and providing an invaluable resource for universities and industries. The FY 2002 funding for this program is $4,160,000 and the DOE contact is Kristin A. Bennett, (301) 903-4269.

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

TECHNOLOGY RESEARCH DIVISION

LABORATORY TECHNOLOGY RESEARCH PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING

252. **ADVANCED PROCESSING TECHNIQUES FOR TAILORED NANOSTRUCTURES IN RARE-EARTH PERMANENT MAGNETS (AL 01 02)**
$198,000
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

253. **DEVELOPMENT OF BISMUTH-BASED SUPERCONDUCTING WIRE WITH IMPROVED CURRENT CARRYING AND FLUX PINNING PROPERTIES (ANL 99 15)**
$96,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Victor Maroni (630) 252-4547

Progress in the commercialization of electric power equipment fabricated with high temperature superconducting materials has been limited by performance issues associated with the maximum achievable engineering critical current density, Je, in long-length composite conductor. One of the most advanced conductors available today for such applications is the silver-clad $(Bi,Pb)_2Sr_2Ca_2Cu_3Oy$ (called Ag/Bi-2223) composite in multifilament form. However, the Je of Ag/Bi-2223 at 77 K in magnetic fields of 1 Tesla or more is not presently adequate for most types of motors, generators, transformers, current limiters, and related power system components. Research is aimed at investigating two new pathways to fabricate the next generation of improved bismuth-based superconducting wire. One pathway is focused on the controlled growth of strong flux pinning centers in Ag/Bi-2223 filaments by the implementation of special heat treatment procedures. These create a transient thermodynamic state that promotes the growth of selected second phase nanocrystallites having the correct size, shape, and spatial distribution to induce strong inter- and intra-granular flux pinning. The second pathway involves reducing the c-axis blocking layer gap (between CuO_2 planes) in layered bismuth cuprates by demonstrating fabrication of the silver-clad $(Bi,Pb,Cd)_1Sr_2Ca_1Cu_2O$ (M-1212) along lines that have been developed for Ag/Bi-2223. The “in-principle” advantage of M-1212 over Bi-2223 stems from the shorter (by ~4 D) blocking gap in M-1212 due to fewer atomic layers in the c-axis repeat unit. From preliminary work, there are existing laboratory scale indications that both pathways can lead to significant improvement in the performance of bismuth-based high temperature composite conductors. The project extends DOE commitments in characterization and design of advanced materials for the acceleration of superconducting technologies to U.S. markets.

Keywords: Superconducting Materials, Silver-Clad $(Bi,Pb)_2Sr_2Ca_2Cu_3Oy$

254. **INTERPLAY BETWEEN INTERFACIAL AND DIELECTRIC AND FERROELECTRIC BEHAVIORS OF BARIUM STRONTIUM TITANATE THIN FILMS (PNL 99 08)**
$118,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNL Contact: Scott Chambers (509) 376-1766

Barium strontium titanate (BST) and related materials are entering commercial use for integrated circuit manufacture as conventional materials reach their fundamental limits. BST films have capacitance, leakage, and related electrical properties that surpass integrated circuit device requirements. One of the most important steps towards understanding the interplay between interfacial properties and dielectric and ferroelectric behaviors of BST ($Ba_{1-x}Sr_xTiO_3$) is the growth of high quality BST films on Si substrates. Successful epitaxial growth of crystalline BST on Si(001) is thought to require the formation of a two-dimensional interfacial silicide layer involving either Ba or Sr as the initial step. Bulk thermodynamics suggests that this thin silicide layer is required to stabilize the interface. The goal of the project is to address two specific issues of significant concern in BST thin-film technology: 1) the effect of interfacial chemistry and stress on the dielectric and ferroelectric properties of BST thin films, and 2) ferroelectric behavior at the nano-scale level. Research is focused on preparation, isolation, and characterization of an ultrathin silicide layer using Sr as the alkaline earth metal. Si(001)-(2x1) surfaces were prepared in ultra high vacuum (UHV) by rapid desorption of the native oxide layer. These surfaces were exposed to Sr from an effusion cell in an oxide MBE chamber as a function of evaporation rate, substrate temperature, and total dose. The resulting interfaces were characterized during growth with reflection high-energy electron diffraction (RHEED), and after growth with low-energy electron diffraction (LEED), X-ray photoemission (XPS), and X-ray photoelectron diffraction (XPD). Additionally, the team is initiating STM investigations to further elucidate this interface structure. Physical and electrical testing of these structures have been performed to determine interface roughness, interface layer formation, interface state density, dielectric properties (permittivity, leakage, etc.), and stability vs. post-growth processing. This project supports DOE's commitment to basic energy sciences in fostering the synthesis, processing, and characterization of advanced materials.

Keywords: BST Thin Films, Dielectric, Ferroelectric Materials, Interfacial Chemistry

255. **ADVANCED COMPUTATIONAL MODELS AND EXPERIMENTS FOR DEFORMATION OF ALUMINUM ALLOYS – PROSPECTS FOR DESIGN (PNL 99 07)**
$90,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNL Contact: M.A. Khaleel (509) 375-2438

Dislocations are the basic lattice line defects in crystalline materials, with defect densities as high as $10^{15}/m^2$. This project aims at understanding their collective and complex nonlinear dynamical behavior by merging a set of highly sophisticated experiments, using computer aided, massive numerical analyses, and experimental data. The project impacts future computational and experimental advances in dislocation theory and elevates prospects for predictive alloy properties control. One motivation for this work is to characterize fabrication and durability characteristics of aluminum tailor welded blanks in order to demonstrate their viability for high volume, low cost stamped automotive panels and structures. Finite Element Modeling is being used to formulate accurate constitutive relations to allow complete description of material response during manufacture. Application of this research to manufacture and design of existing and new lightweight Al materials supports DOE's initiatives in high performance computing.

Keywords: Aluminum Alloys, Dislocation Phenomena, Predictive Properties Control

256. **NEAR-FRICTIONLESS CARBON COATINGS (ANL 98 03)**
$19,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Ali Erdemir (630) 252-6571

Numerous industrial applications involve the use of mechanical devices containing components that slide or roll against one another. The efficiency and durability of these components are often limited by the friction and wear properties of the materials used to fabricate the components. For example, Diesel Technology Company (DTC) and Stirling Thermal Motors (STM) develop advanced energy conversion systems and engine components that will contribute significantly to reducing oil imports and improving air quality by reducing engine emissions. Fuel injection systems being designed and developed by Diesel Technology for use in heavy-duty diesel engines will require tighter tolerances to run on low-lubricity fuels at higher operating pressures needed to achieve emissions and efficiency goals. Since materials used in current fuel injection systems will not survive under these aggravated conditions, new materials and/or coatings are needed. Similarly, Stirling engines being designed by Stirling Thermal Motors will operate under tribological conditions (e.g., speeds, temperatures, loads, and working fluids) not commonly encountered, and will require advanced materials, coatings, and lubricants to ensure long-term durability. Argonne will work with Front-Edge Technologies (FET) to commercialize Argonne's technology for fuel injection systems and Stirling engine components being developed by DTC and STM. The objectives of this project are to: 1) advance the basic understanding of the physical/chemical and tribological processes controlling the friction and wear behavior of the new carbon films 2) demonstrate the ability of these coatings to improve the friction and wear performance of materials and components being developed by Diesel Technology and Stirling Thermal Motors, and 3) demonstrate that the coating technology can be scaled-up to coat large numbers of components on a cost-competitive basis. If successful, the NFC technology will have a significant impact not only on the technology being pursued by DTC and STM, but also in other applications found in the aerospace, biomedical, and manufacturing sectors. It builds on expertise at Argonne in tribology, coatings, and materials characterization. This project supports DOE missions in advanced materials and sustainable environments, reducing U.S. dependence on foreign oil imports, and improving U.S. air quality. This project won an R&D 100 Award in 1998.

Keywords: Carbon Coatings, Friction and Wear, Fuel Injection, New Materials, Coatings, Tribology

257. **INTERFACIAL PROPERTIES OF ELECTRON BEAM CURED COMPOSITES (ORNL 99 08)**
$105,000
DOE Contact: Samuel J. Barish (301) 903-2917
ORNL Contact: Christopher Janke (423) 574-9247

Electron Beam curing of composites and adhesives is a nonthermal, nonautoclave curing process which offers substantially reduced manufacturing costs and curing times, improvements in part quality and performance, reduced environmental and health concerns, and improvements in material handling, as compared to conventional thermal curing. As satisfactory properties of electron beam cured composites are achieved, U.S. industry expects rapid implementation of these materials for making better, less expensive, and lightweight airplanes, spacecraft, and automobiles. Previous research on electron beam cured composites has shown that interface dependent properties, such as composite interlaminar shear strength, are generally lower than those of high performance, autoclave cured composites. A primary objective of this project is to determine the chemical, physical, and/or mechanical mechanisms responsible for poor adhesion between carbon fibers and epoxy resins subjected to electron beam processing. Another important objective is to optimize electron beam compatible carbon fiber surface treatments, chemical agents, modified radiation curable epoxy resin systems, and improved fabrication and processing methods for producing electron beam cured composites having excellent interfacial properties. Currently, work is focused on characterization of the carbon fiber-epoxy resin interface and identification of the critical radiation processing parameters that influence the properties of electron beam cured composites. Additionally, various chemical agents, including coupling agents and reactive finishes, which are specifically designed to improve the fiber-resin adhesion properties, are being evaluated. The project complements DOE investments in advanced materials research, and research on energy efficiency and environmental stewardship.

Keywords: Electron Beam Processing, Electron Beam Cured Composites and Adhesives

258. **PHOTOCATALYTIC METAL DEPOSITION FOR NANOLITHOGRAPHY (ANL 99 13)**
$205,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Tijana Rajh (630) 252-3542

A major technical impediment for the development of mesoscopic scale electronic devices is obtaining molecular scale conducting patterns. Based on the parameters that are optimized in highly efficient photochemical energy conversion in natural photosynthesis, Argonne National Laboratory has developed a new mask-less photoelectrochemical method for depositing conductive metal patterns with nanometer scale precision. This technology will enable the rapid prototyping and manufacturing of mesoscopic electronics and offers the potential of low-cost small batch manufacturing and unparalleled levels of electronic integration. This new technology is being used to fabricate miniaturized (ultimate resolution limit of 1 nm) and rugged electrical interconnects and biomolecular electronic devices on any surface or in solution. This project will enable the 3-D integration of passive and active components of mesoscopic integrated conformal electronics. In addition, the technology provides a unique advantage compared to other electronic technologies, because the semiconductor substrate (precursor) can also perform active function in the bioelectronic device. Conductor precursors, semiconductor metal oxide nanoparticles modified with chelating agents, that bind metal cations (copper, silver, and gold), will be synthesized. Biological templates will be used to self-assemble conductor precursors in order to achieve spacial resolution via photocatalysis. The fast photoresponse of semiconductor nanodots also provides high time resolution. Based on a fundamental understanding of electron transfer reactions in this biomimetic approach, precursor formulations will be developed and characterized for photoelectrochemical response, redox stability, and mechanical properties. Precursors will be deposited on a range of substrates (silicon, glass, plastic, metals, ceramics, etc.) or in solution. Conductive patterns formed by catalytic semiconductor assisted solid state deposition of copper, silver, or gold will be studied as a function of nanoparticle size, reduction technique, and nanoparticle-chelate association complex. Interconnects and biomolecular assemblies will be studied to ascertain morphology, function, and 3-D characterization as a function of processing methodology. The technology developed in this project is an extension of DOE's efforts to promote characterization of materials useful to nanotechnology.

Keywords: Metal Deposition, Nanolithography, Self Assembly, Photocatalysis

259. **LOW-COST, HIGH-PERFORMANCE YBCO CONDUCTORS (ORNL 01 06)**
$189,000
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

260. NANOFABRICATION OF ADVANCED DIAMOND TOOLS (LBNL 01 03)

$150,000
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

261. **DEVELOPMENT OF A HIGH-EFFICIENCY ROTARY MAGNETOCALORIC REFRIGERATOR PROTOTYPE (AL 99 02)**
$125,000
DOE Contact: Samuel J. Barish (301) 903-2917
AL Contact: K. A. Gschneidner, Jr. (515) 294-7931

Magnetic refrigeration is based on the magnetocaloric effect—the ability of some materials to heat up when magnetized and cool when removed from the magnetic field. Using these materials as refrigerants would provide an environmentally friendly alternative to the volatile liquid chemicals, such as chlorofluorocarbons and hydrochlorofluorocarbons, used in traditional vapor-cycle cooling systeThe new materials have two advantages over existing magnetic coolants: they exhibit a giant magnetocaloric effect, and their operating temperature can be tuned from about 30K (-400˚F) to about 290K (65˚F) by adjusting the ratio of silicon to germanium—the more germanium, the lower the temperature. The efficiency of the new materials make magnetic refrigeration even more competitive with conventional gas-compression technology by replacing complex and costly superconducting magnets with permanent magnets in refrigerator designs. The elimination of superconducting magnets may also open the way for small-scale applications of this technology, such as climate control in cars and homes, and in home refrigerators and freezers. In addition, G. Schneidner says, “the discovery may also launch totally new applications for efficient refrigerators at very low refrigeration powers since gas compression technology cannot be scaled down to such low cooling powers and since thermoelectric cooling is very inefficient (30 times less than magnetic refrigerants).” The first gadolinium-based magnetic refrigerator has been demonstrated. The refrigerator has been operating for over six months, which far exceeds the few hours or days of operation recorded by similar units. In addition, the unit has achieved cooling power 20 to 1,000 times greater than previous units. Currently, the team is working to find practical means of processing the new materials to construct and test a variety of magnetic refrigerators, which span temperatures from 20K (-425˚F) to 300K (80˚F) and have cooling powers ranging from one watt to 50,000 watts. The project transfers DOE’s investments in materials research to research in energy efficiency through reduction in operating costs in air conditioning and refrigeration.

Keywords: Magnetocaloric Effect, Magnetocaloric Refrigeration, Gadolinium-Based Magnetic Materials

262. **DIRECT CASTING OF TITANIUM ALLOY WIRE FOR LOW-COST AEROSPACE AND AUTOMOTIVE FASTENERS (PNL 99 02)**
$73,000
DOE Contact: Samuel J. Barish (301) 903-2917
PNNL Contact: Mark Smith (509) 376-2847

Current wire production methods require large ingots to undergo multiple reduction steps until a diameter of 7mm or less is obtained. The reduction steps are energy intensive, require expensive equipment, and result in the generation of scrap materials and undesirable etchant and lubricant waste. Economic analysis indicates that direct casting of a titanium wire to a diameter slightly larger than the desired final product, followed by relatively small final reduction steps, will result in significant savings to the aerospace industry and other titanium wire/rod users.

The direct casting process involves the use of a titanium core wire to serve as the carrier substrate onto which titanium will be cast and solidified at high feed rates. The objectives of the project include the development of unique atmosphere-controlled casting equipment, the application of thermal models to optimize the design and operation of the casting process, and extensive materials testing and characterization to establish the capability of the process to match properties produced by conventional processing. The project extends DOE investments in materials characterization to develop process technologies which further reduction of industrial waste emissions.

Keywords: Titanium Alloy Wire, Casting Processes

263. **NONCONSUMABLE METAL ANODES FOR PRIMARY MAGNESIUM PRODUCTION (ANL 98 05)**
$110,000
DOE Contact: Samuel J. Barish (301) 903-2917
ANL Contact: Michael J. Pellin (630) 252-3510

This project will develop a nonconsumable metal anode to replace consumable carbon anodes now used in commercial electrolysis cells for primary magnesium production. The use and manufacture of consumable carbon anodes, which must be constantly replaced, is costly, energy consuming, and occasions unwanted gaseous emissions such as CO_2 and HCl. In support of the DOE mission for energy efficient, environmentally sound industrial processes, ANL has identified certain metal alloys that are promising candidate materials for nonconsumable anodes. Such alloys form self-limiting surface oxide films that are thin enough to allow current to pass, yet thick enough to prevent attack of the underlying metal. These alloys are dynamic in that the more volatile, reactive components segregate to the surface at rates sufficient to reform the protective film as it dissolves in the chloride melt. The project will form surface films on candidate alloys and investigate them using surface analysis instruments and techniques. Promising alloys will be tested as anodes in bench-scale magnesium electrolysis cells. Cell operation will be monitored and interrupted at key points to remove the anode and investigate its surface film. If desirable, the anode film thickness and strain during electrolysis in specially designed cells will be studied. Alloys identified as optimal will be subject to long-term bench-scale tests by Dow Chemical Company, and then tested in full-scale cells at Dow's production facility in Freeport, Texas. Successful completion of this work will result in increased U.S. competitiveness and lower magnesium prices which would, for example, allow magnesium to be used more widely in the transportation sector, resulting in lower costs there. If successful, stable anodes would reduce the operation cost of making magnesium by 20-30 percent and eliminate the emission of CO_2 and other halocarbon gases during magnesium production by eliminating the need for carbon anodes, now used to produce magnesium electrolytically. Moreover, this work will illuminate the mechanisms associated with film formation on alloys. An understanding of these mechanisms (e.g., surface segregation, near surface diffusion) will provide the basis for developing a new class of corrosion resistant materials that can find application in harsh chemical environments, for example as nonconsumable anodes for aluminum production.

Keywords: Magnesium Production, Metal Anodes, Metal Alloy, CO_2 Emissions, Corrosion Resistant, Film Formation

264. **OPTIMIZED CATALYSTS FOR THE CRACKING OF HEAVIER PETROLEUM FEEDSTOCKS (LBNL 99 01)**
$67,000
DOE Contact: Samuel J. Barish (301) 903-2927
LBL Contact: Gabor Somorjai (510) 486-4831

Catalysts lower the energy required for chemical reactions to proceed and are widely used in petroleum refining and chemical manufacturing. The useful lifetime and, thus, the value of an industrial catalyst are limited by a process known as deactivation in which the efficiency of the catalyst declines over time. Understanding the deactivation process is essential for developing new catalysts with longer useful lifetimes. There are two industrially important catalytic systems under study at present. In the first study, zeolite-based catalysts are being developed to remove undesired sulfur compounds from gasoline. The goal of this project is to evaluate the mechanism by which sulfur is adsorbed on the catalyst. Of particular interest is the identification of catalyst "active sites" that actually interact with the sulfur. This is done by spectroscopically monitoring the identity of the surface species under reaction conditions. The second system under study is the "reforming" reactions of n-hexane and n-heptane with hydrogen that produce high octane gasoline by converting the reactants to benzene and toluene. Deactivation in these catalysts proceeds via "coking," the buildup and polymerization of carbonaceous reaction byproducts on the surface of the catalyst. The vibrational spectra of these byproducts will be obtained by UV-Raman spectroscopy for identification purposes. Ultraviolet excitation is required in this case to avoid interference from black body radiation from the hot catalyst material. Identification of problematic surface species will allow determination of the precise mechanism by which deactivation occurs in this system. These improvements will have a major impact on the efficiency of petroleum refining and gasoline production. The new surface science tools under development will have applicability to general studies in catalysis and surface science and support the DOE's mission in design and characterization of advanced materials.

Keywords: In-Situ Surface UV-Raman Spectroscopy, Catalytic Surfaces, Catalyst Deactivation, Zeolite Based Materials

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

Silicon Carbide High Temperature Dynamic Pressure Gauge - DOE contact Richard J. Dunst, (412) 386-6694; Busek Company, Inc. contact Judy Budny, (508) 655-5565

Turbine Blade Emissivity Sensor - DOE contact Charles T. Alsup, (304) 284-5432; En'urga, Inc. contact Vinoo Narayan, (765) 497-3269

Development of Robust NO_x Monitor - DOE contact Richard J. Dunst, (412) 386-6694; Nextech Materials, Ltd. contact William J. Dawson, (614) 842-6606

Amorphous, Non-Oxide Seals, Derived from Organic Precursors, for Solid Oxide Fuel Cells - DOE contact Lane Wilson, (304) 285-1336; Ceramatec, Inc. contact Dr. Michael A. Keene, (801) 978-2152

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 William J. Dawson, (614) 842-6606

Internal Pipe Repair System - DOE contact Magda Rivera, (304) 285-1359; Foster-miller, Inc. contact Mr. Ross R. Olander, (781) 684-4242

Assure Natural Gas and Oil Pipeline Reliability by Cost-Effective, High-Performance Thermoplastic Liners - DOE contact Magda Rivera, (304) 285-1359; Frontier Performance Polymers Corporation contact Dr. Jerry S. Chung, (973) 331-0923

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

Catalysts and Membrane for Selective Methane Oxidative Dimerization - DOE contact Charles Taylor, (412) 386-6058; Eltron Research, Inc. contact Ms. Eileen E. Sammells, (303) 530-0263

High Efficiency Amorphous and Microcrystalline Silicon Based Double-Junction Solar Cells Made with Very-High-Frequency Glow Discharge - DOE contact Satyen Deb, (303) 384-6405; United Solar Systems Corp. contact J. Vanaharam, (248) 364-5611

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

The Development of a Low-Cost Separator with Improved Performance - DOE contact Jim Barnes, (202) 586-5657; Yardney Technical Products, Inc. contact Vincent Yevoli, (860) 599-1100

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

Monomer-Excimer Phosphorescent White OLEDS for General Lighting - DOE contact James Brodrick, (202) 586-1856; Universal Display Corporation contact Janice K. Mahon, (609) 671-0980

White Illumination Sources Using Striped Phosphorescent OLEDs - DOE contact James Brodrick, (202) 586-1856; Universal Display Corporation contact Janice K. Mahon, (609) 671-0980

An Approach for Reducing Wind Turbine Tower Weight by 70 Percent by Combining an Innovative On-Site Manufacturing Method with a Novel Tower Design - DOE contact John Cadogan, (202) 586-1991; Composite Support & Solutions, Inc. contact Dr. Clement Hiel, (310) 265-0850

Development of a Low Wind Turbine Blade Making Optimal Use of Carbon Fiber Composites - DOE contact John Cadogan, (202) 586-1991; Global Energy Concepts, Llc contact Robert Poore, (425) 822-9008

Utilization of Isotruss Technology in Taller Wind Turbine Towers - DOE contact John Cadogan, (202) 586-1991; Wasatch Valley Technologies, Llc contact Christopher Derrington, (801) 264-5600

Transformer Ratio Enhancement Experiment for Next Generation Dielectric Wakefield Accelerators - DOE contact Jerry Peters, (301) 903-3233; Euclid Concepts Llc contact Dr. A.D. Kanereykin, (440) 519-0410

Inexpensive High Quality Electron Sources - DOE contact Jerry Peters, (301) 903-3233; Genvac Aerospace contact Carole Ream, (440) 646-9986

Continuous Formation of Ta Barrier and Cu Sheath of Nb_3Sn Subelements - DOE contact Jerry Peters, (301) 903-3233; Accelerator Technology Corporation contact Dr. Peter McIntyre, (979) 255-5531

Concentric Tilted Double-Helix Dipole Magnets - DOE contact Jerry Peters, (301) 903-3233; Advanced Magnet Laboratory, Inc. contact Mark Senti, (321) 728-7543

Multifilament Extrusion Cuprate Superconductors - DOE contact Jerry Peters, (301) 903-3233; Alchemet, Inc. contact Katherine L. Miller, (610) 566-5964

Advanced, High-Filament-Count, Nb_3Al, Jelly-Roll Strand for Accelerator Applications - DOE contact Jerry Peters, (301) 903-3233; Hyper Tech Research Inc. contact Michael Tomsic, (937) 332-0348

Eliminating a Major Cause of Wire Drawing Breakage in A-15 High-Field Superconductors - DOE contact Jerry Peters, (301) 903-3233; Innovare, Inc. contact Dr. Alfred R. Austen, (610) 837-8830

Optimization and Commercialization of the Cable-In-Tube Approach to Fabricating High Performance Nb_3Sn Wires - DOE contact Jerry Peters, (301) 903-3233; Superconducting Systems, Inc. contact Dr. Shanhin Pourrahimi, (781) 642-6702

High Current Density (Jc), Low AC Loss, Low Cost Internal-Tin Superconductors - DOE contact Jerry Peters, (301) 903-3233; Supergenics contact Bruce Zeitlin, (941) 349-0930

Hybrid Electrochemical - Electrolytic Capacitor for Next-Generation Electron-Positron Linear Collider - DOE contact Jerry Peters, (301) 903-3233; Giner Electrochemical Systems, LLC contact Dr. Anthony J. Vaccaro, (781) 529-0504

Microwave Component Fabrication using the Fast Combustion Driven Compaction Process - DOE contact Jerry Peters, (301) 903-3233; Utron, Inc. contact Dr. F. Douglas Witherspoon, (703) 369-5552

A High Thermal Performance, Self-Contained Heat Extraction System suited to Highly Distributed Heat Sources, with Premise Based on Ultra-Lightweight Considerations - DOE contact Michael P. Procario, (301) 903-2890; Allcomp, Inc. contact Wei Shih, (626) 369-4572

Cylindrical Electrode-Less Gas Electron Multiplier - DOE contact Michael P. Procario, (301)903-2890; Ion Optics, Inc. contact James C. Louney, (781) 788-8777

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

Radiation Hard Lead Zirconium Titanium (PZT) for Ferroelectric and Plezoelectric Devices - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Structured Materials Industries, Inc. contact Joseph D. Cuchiaro, (719) 260-9589

Innovative Helium-Cooled Tungsten PFCs - DOE contact Sam E. Berk, (301) 903-4171; Plasma Processes, Inc. contact Timothy McKechnie, (256) 851-7653

Insulators and Materials for Close-Spaced Thermoelectric Modules - DOE contact Robert Wiley, (301) 903-2884; Hi-z Technology, Inc. contact Norbert B. Elsner, (858) 695-6660

Separation and Enrichment of Xenon in Air - DOE contact Ken Quitoriano, (925) 423-6331; Membrane Technology And Research, Inc. (MTR) contact Elizabeth Weiss, (650) 328-2228

A Small Seismic Accelerometer Utilizing Single Crystal Piezoelectric Material - DOE contact Ken Quitoriano, (925) 423-6331; Wilcoxon Research, Inc. contact David L. Spilis, (301) 216-3016

High Performance Thermo-Electrically-Cooled LWIR Mercury Cadmium Telluride Detectors - DOE contact Ken Quitoriano, (925) 423-6331; Fermionics Corporation contact Dr. C. C. Wang, (805) 582-0155

Nano Liter Scale Blood Sampling and Analysis System - DOE contact Dean Cole, (301) 903-3268; Phoenix Bioscience contact Kumar Subramanian, (925) 858-0484

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

PHASE II (FIRST YEAR)

A High-Power, Ceramic, RF Generator and Extractor - DOE contact Jerry Peters, (301) 903-3233; 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 Jerry Peters, (301) 903-3233; Omega-p, Inc. contact 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 Jerry Peters, (301) 903-3233; Supergenics contact 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 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 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 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 Clifton H. Brown, (303) 792-5615

Control of Catalyst Poisons from Coal Gasifiers - DOE contact Bob Kornosky, (412) 386-4521; TDA Research, Inc. contact Michael Karpuk, (303) 940-2301

High-Temperature Highly-Efficient Ceramic Heat Exchanger - DOE contact Richard J. Dunst, (412) 386-6694; Ceramatec, Inc. contact Dale M. Taylor, (801) 978-2132

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (SECOND YEAR)

Non-Linear Optical Devices for High Performance Networking, Computing and Telecommunication Routing and Modulating - DOE contact George Seweryniak, (301) 903-0071; Ionic Systems, Inc. contact Constance Eve Teague, (408) 885-0800

Advanced Geothermal Optical Transducer (AGOT) - DOE contact Raymond J. LaSala, (202) 586-4198; LEL Corporation contact Piedao H. Liucci, (201) 569-8641

Fast-Response, Two-Dimensional Detector for Epithermal Neutron Detection with Adjustable Shape - DOE contact Helen Kerch, (301) 903-2346; Nova Scientific, Inc. contact Dr. Paul L. White, (508) 347-7679

Ceramic Appliques for the Production of Supported Thin-Film Catalytic Membrane Reactors - DOE contact Charlie Russomanno, (202) 586-7543; Eltron Research, Inc. contact Eileen E. Sammells, (303) 530-0263

Affinity Ceramic Membranes with Carbon Dioxide Transport Channel - DOE contact Charlie Russomanno, (202) 586-7543; Media and Process Technology, Inc. contact Dr. Paul K.T. Liu, (412) 826-3721

Photocatalytic Membranes for Producing Ultrapure Water - DOE contact Charlie Russomanno, (202) 586-7543; Technology Assessment & Transfer, Inc. contact Sharon S. Fehrenbacher, (410) 224-3710

Novel Membrane Reactor for Fischer-Tropsch Synthesis - DOE contact Charlie Russomanno, (202) 586-7543; CeraMem Corporation contact Dr. Robert Goldsmith, (781) 899-4495

Fast, Low-Noise Readout Chip for Avalanche Photodiode Arrays for Use in Positron-Emission Tomography Imaging - DOE contact Prem Srivastava, (301) 903-4071; Nova R & D, Inc. contact Raymond B. Pifer, (909) 781-7332

Miniature Electrochemical Carbon Dioxide Detector - DOE contact Roger Dahlman, (301) 903-4951; Superior Sensing Solutions contact Michael J. Newman, (303) 702-1672

An Innovative Ultramicroelectrode Array for Field-Deployable Trace Metal Analysis - DOE contact Paul Bayer, (301) 903-5324; Lynntech, Inc. contact Dr. G. Duncan Hitchens, (979) 693-0017

Novel Joining Technique for Oxide-Dispersion Strengthened Iron Aluminide Alloys - DOE contact Richard Read, (412) 386-5721; Materials & Electrochemical Research (MER) Corp. contact Dr. R. O. Loutfy, (520) 574-1980

A Metallic Interconnect for Intermediate Temperature, Planar, Solid Oxide Fuel Cells - DOE contact Wayne Surdoval, (412) 386-6002; Materials and Systems Research, Inc. contact Dr. Dinesh K. Shetty, (801) 530-4987

Tailorable, Inexpensive Carbon Foam Electrodes for High-Efficiency Fuel Cell and Electrochemical Applications - DOE contact Richard Read, (412) 386-5721; Touchstone Research Laboratory, Ltd. contact Brian E. Joseph, (304) 547-5800

Advanced Cathode Structure for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cells - DOE contact Ronald J. Fiskum, (202) 586-9154; FuelCell Energy, Inc. contact Dr. Hans Maru, (203) 825-6006

Efficient Incandescent Lighting Based on Selective Thermal Emitters - DOE contact John Ryan, (202) 586-9130; Foster-Miller, Inc. contact Adi R. Guzdar, (781) 684-4239

'On Chip' Smart Sensor Array and Control Teleplatform for Thermophotovoltaic Cell Manufacturing Applications - DOE contact Alec Bulawka, (202) 586-5633; ARSECO contact Marine Boyadzhyan, (818) 249-6362

Infrared Focal Plane Array with Fast Shuttering - DOE contact Eric Sander, (202) 586-5852; Princeton Scientific Instruments, Inc. contact John L. Lowrance, (732) 274-0774

Linear Avalanche Photodiode Detector Arrays for Gated Spectroscopy with Single-Photon Sensitivity - DOE contact Eric Sander, (202) 586-5852; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

Development of a Large-Area Mercuric Iodide Photodetector for Scintillation Spectroscopy - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Constellation Technology Corporation contact Charles Settgast, (727) 547-0600

Segmented, Deep-Sensitive-Depth Silicon Radiation Detectors - DOE contact Jehanne Simon-Gillo, (301) 903-1455; IntraSpec, Inc. contact John Walter, (865) 483-1394

Micromachined Silicon, Large Area X-ray Detector - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Physical Optics Corporation contact Gordon Drew, (310) 320-3088

Cost Reduction Techniques for Powder-in-Tube Niobium-Tin Superconductors - DOE contact Jerry Peters, (301) 903-5228; Supercon, Inc. contact Elaine Tarkiainen, (508) 842-0174

Flexible Niobium-Tin Cables Suitable to React-then-Wind Approach to Fabricating Accelerator Magnets - DOE contact Jerry Peters, (301) 903-5228; Superconducting Systems, Inc. contact Dr. Shanin Pourrahimi, (781) 642-6702

Novel Avalanche Photodiode Arrays for Scintillating Fiber Readout - DOE contact Michael P. Procario, (301) 903-2890; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

Manufacturing of Robust Ceramic/Metal Joints for Alkali Metal Thermal-to-Electric Converters - DOE contact Lisa C. Herrera, (301) 903-8218; Triton Systems, Inc. contact Ross Haghighat, (978) 250-4200

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Multilayer Composite Membranes for Upgrading Acid-Rich Natural Gas - DOE contact Tony Zammerilli, (304) 285-4641; Membrane Technology And Research, Inc. (MTR) contact Elizabeth Weiss, (650) 328-2228

Low-Temperature, Solid Oxide Fuel Cell Cathode Development - DOE contact Lane Wilson, (304) 285-1336; Ceramatec, Inc. contact Dr. Michael Keene, (801) 978-2152

Use of Graphite Nanofibers as a Catalyst for the Synthesis of Styrene - DOE contact Charlie Russomanno, (202) 586-7543; Catalytic Materials, Ltd. contact Dr. Nelly Rodriguez, (508) 893-9561

Modeling of Copper-Indium-Gallium Diselenide for Advanced Thin-Film Photovoltaic Devices - DOE contact Satyen Deb, (303) 384-6405; Helio Volt Corporation contact Dr. Ronald P. Gale, (617) 962-2608

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

A Multi-Megawatt Continuous Wave RF Window for Particle Accelerator Applications - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Tunnel Dust, Inc. contact Roisin F. Preble, (757) 898-3373

An IR Imaging and Spectral Diagnostic System for Alcator C-Mod - DOE contact Charles Finfgeld, (301) 903-3423; Science Research Laboratory, Inc. contact Dr. Jonah Jacob, (617) 547-1122

A Solid-State Irradiance Calibrator for Field Use - DOE contact Michael Huesemann, (360) 681-3618; Yankee Environmental Systems, Inc. contact Cynthia A. Cote, (413) 863-0200

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE II (FIRST YEAR)

Doppler Laser Radar for Non-Intrusive Liquid Metal Flow Characterization - DOE contact Sam E. Berk, (301) 903-4171; Think Tank, Inc. contact Dr. Madhavan M. Menon, (865) 966-6200

Multi-Megawatt Circulator for TE01 Waveguide - DOE contact Jerry Peters, (301) 903-3233; Calabazas Creek Research contact Dr. Lawrence Ives, (408) 741-8680

Active Vibration Control of NLC Magnets - DOE contact Jerry Peters, (301) 903-3233; 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 Shelby J. Morris Jr., (757) 850-8679

X-ray Diagnostics for High-Temperature Superconductor Processing - DOE contact David Welch, (631) 344-3517; Aracor contact 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 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 PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE II (SECOND YEAR)

Utilization of Hydrocarbon Fuels in Low-Temperature Solid Oxide Fuel Cells - DOE contact Wayne Surdoval, (412) 386-6002; Applied Thin Films, Inc. contact Derrick Calandra, (847) 467-6877

Thin Alternatives to Braided Glass Insulation for Low-Temperature Superconducting Wire - DOE contact Jerry Peters, (301) 903-5228; Microcoating Technologies contact Jeffrey Moore, (678) 287-2400

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Embedded Sensors in Turbine Systems by Direct Write Thermal Spray Technology - DOE contact Charles T. Alsup, (304) 284-5432; Mesoscribe Technologies, Inc. contact Richard Gambino, (631) 632-9513

Contamination Resistant Anodes for Intermediate Temperature Solid Oxide Fuel Cells - DOE contact Lane Wilson, (304) 285-1336; Eltron Research, Inc. contact Eileen E. Sammells, (303) 530-0263

CU-SDC Nanostructural Electrodes as Coking-Resistant Anodes for Intermediate-Temperature SOFCS - DOE contact Lane Wilson, (304) 285-1336; Microcoating Technologies contact David L. Motley, (678) 287-2445

Low-Cost Protective Layer Coatings on Thermal Barrier Coatings via CCVD - DOE contact Udaya Rao, (412) 386-4743; Microcoating Technologies contact David L. Motley, (678) 287-2445

A Commercially Viable Carbon Molecular Sieve Membrane for Subquality Natural Gas - DOE contact Tony Zammerilli, (304) 285-4641; Media And Process Technology, Inc. contact Dr. Paul KT Liu, (412) 826-3721

Catalyst to Improve Small-Scale Claus Plants - DOE contact Tony Zammerilli, (304) 285-4641; Tda Research, Inc. contact 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

Advanced Structural Carbon-Supported Catalysts for Industrial Polymer Synthesis - DOE contact Charlie Russomanno, (202) 586-7543; Environmental And Life Support Technologies, Inc. contact Clifford D. Jolly, (303) 840-4221

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

Solid-Acid Catalyst for Refinery Alkylation - DOE contact Charlie Russomanno, (202) 586-7543; Exelus, Inc. contact Mitrajit Mukherjee, (973) 740-2350

Structured Catalyst for Exothermic Reactions - DOE contact Charlie Russomanno, (202) 586-7543; Exelus, Inc. contact Mitrajit Mukherjee, (973) 740-2350

Development of Ion Beam Techniques for Layer Splitting of Oxide Materials - DOE contact Tony Haynes, (865) 576-2858; Ues, Inc. contact Francis F. Williams, Jr., (937) 426-6900

A Novel Technique to Produce Ultra-Porous Metallic Foams through Thermal Reduction of Nano-Particle Oxide - DOE contact Mike Kassner, (541) 737-7023; Micropyretics Heaters International, Inc. contact Dr. A. Vissa, (513) 772-0404

Novel High Temperature Polymer Substrate for Low Cost High Efficiency Thin Film CIGS Solar Cells - DOE contact Satyen Deb, (303) 384-6405; Foster-miller, Inc. contact Ross R. Olander, (781) 684-4242

Non-Vacuum Techniques for Front and Back contacts for CIGS Solar Cells - DOE contact Satyen Deb, (303) 384-6405; International Solar Electric Technology, Inc. contact Dr. Vijay K. Kapur, (310) 216-1423

Transparent Conducting Oxide Films with High Refractive Index - DOE contact Satyen Deb, (303) 384-6405; Microcoating Technologies contact David L. Motley, (678) 287-2445

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

Polymer and Gel Electrolyte for Lithium Sulfur Batteries - DOE contact Jim Barnes, (202) 586-5657; Moltech Corporation contact Dr.Jim Akridge, (520) 799-7516

The Development of a Polyvalent Battery System - DOE contact Jim Barnes, (202) 586-5657; Yardney Technical Products, Inc. contact Vince Yevoli, (860) 599-1100

Synthesis & Integration of Quantum Confined Atom (QCA) Nanophosphor Based Down Converter for AlInGaN-Based High Luminous Efficiency White-Light LED Lamps - DOE contact Eric Jones, (505) 844-8752; Nanocrystals Technology, Ltd. contact Dr. Rameshwar N. Bhargava, (914) 923-1142

General Illumination Using Dye-Doped Polymer Light Emitting Devices - DOE contact James Brodrick, (202) 586-1856; Intelligent Optical Systems, Inc. contact Dr. Ashutosh Sharma, (310) 530-7130

Nanomaterials-Based Electrodes for High Charge Rate Energy Storage Devices of HEVs - DOE contact Imre Gyuk, (202) 586-1482; Nanopowder Enterprises, Inc. contact Dr. Gary S. Tompa, (732) 885-5909

Supported Urania Catalysts for Fatty Acid Methyl Ester Dehydrogenation - DOE contact Amy Miranda, (202) 586-6471; Ceramem Corporation contact Dr. Richard Higgins, (781) 899-4495

Three-Dimension Woven Carbon-Glass Hybrid Wind Turbine Blades - DOE contact John Cadogan, (202) 586-1991; 3tex, Inc. contact R. Bradley Lienhart, (919) 481-2500

PIT Nb_3Sn Superconducting Strands Based on a Modified Powder/Tube Reaction Route - DOE contact Jerry Peters, (301) 903-3233; Hyper Tech Research Inc. contact Michael Tomsic, (937) 332-0348

Non-Copper J_c of 2800 A/mm^2 through Optimization of PIT Nb_3Sn Conductor Design - DOE contact Jerry Peters, (301) 903-3233; Supercon, Inc. contact Terence Wong, (508) 842-0174

An Elemental Powder Approach for High Performance Nb_3Sn Superconductors - DOE contact Jerry Peters, (301) 903-3233; Supercon, Inc. contact Terence Wong, (508) 842-0174

Feasibility of Cost Effective, Long Length, BSCCO 2212 Round Wires, for Very High Field Magnets, Beyond 12 Tesla at 4.2 Kelvin - DOE contact Jerry Peters, (301) 903-3233; Superconductive Components, Inc. contact J.R. Gaines, Jr., (614) 486-0261

A New Method for Depositing Niobium Films for Niobium/Copper Cavities - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Tunnel Dust, Inc. contact Roisin F. Preble, (757) 898-3373

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 Superior Scintillator Material for High Resolution X-ray Detectors - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Nanomat, Inc. contact Shree Kumar, (724) 861-6125

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 Sam E. Berk, (301) 903-4171; Plasma Processes, Inc. contact Timothy McKechnie, (256) 851-7653

High-Strength, High-Conductivity Composite for Plasma Facing Applications - DOE contact Sam E. Berk, (301) 903-4171; Supercon, Inc. contact Terence Wong, (508) 842-0174

Rugged Packaging for Damage Resistant Inertial Fusion Energy Optics - DOE contact Gene Nardella, (301) 903-4956; Pvd Products, Inc. contact Dr. James A. Greer, (978) 694-9455

Low Cost Materials for Neutron Absorption in Generation IV Nuclear Power Systems - DOE contact Madeline Feltus, (301) 903-2308; Powdermet, Inc. contact Andrew Sherman, (818) 768-6420

High Resolution Gamma Ray Spectrometer for Nuclear Non-Proliferation - DOE contact Ken Quitoriano, (925) 423-6331; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

Growth of a New Mid-IR Laser Crystal - DOE contact Ken Quitoriano, (925) 423-6331; Ceramare Corporation contact Dr. Larry E. McCandlish, (732) 937-8260

Ultrapurification, Crystal Growth, and Characterization of Rare-Earth Doped KPb_2Br_5 for Mid-Infared Lasers - DOE contact Ken Quitoriano, (925) 423-6331; Eic Laboratories, Inc. contact Dr. R. David Rauh, (781) 769-9450

Induim Arsenide Antimonide Very Long Wavelength Photodiodes for Near Room Temperature Operation - DOE contact Ken Quitoriano, (925) 423-6331; Svt Associates contact Jane Marks, (952) 934-2100

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (FIRST 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 Eileen E. Sammells, (303) 530-0263

Ultra-Thin Optical Diagnostic Filters for Plasma Wakefield Accelerators - DOE contact Jerry Peters, (301) 903-3233; Luxel Corporation contact 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 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 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 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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (SECOND YEAR)

The Development and Demonstration of Reliable Adherent Metalization of AIN - DOE contact Samuel Barish, (301) 903-2917; MER Corporation contact Dr. R.O. Loutfy, (520) 574-1980

Novel Lithium-Ion Conducting Polymer Electrolytes for Lithium-Ion Batteries - DOE contact Susan Rogers, (202) 586-8997; Eltron Research, Inc. contact Eileen Sammells, (303) 530-0263

Synthesis of New Solid Polymer Electrolytes - DOE contact Susan Rogers, (202) 586-8997; TPL, Inc. contact H.M. Stoller, (505) 342-4412

Membranes for Reverse Organic-Air Separations - DOE contact Charlie Russomanno, (202) 586-7543; Compact Membrane Systems, Inc. contact Glenn Walker, (937) 252-8969

Hydrogen Recovery Process Using New Membrane Materials - DOE contact Charlie Russomanno, (202) 586-7543; Membrane Technology and Research, Inc. contact E.G. Weiss, (650) 328-2228

New Boronated Amino Acids for Neutron Capture Therapy - DOE contact Peter Kirchner, (301) 903-9106; BioNeutrics, Inc. contact Larry Tummel, (865) 675-5627

Low-Cost Arc Process to Produce Single-Walled Nano-Tubes Using Coal-Based Starting Materials - DOE contact Neil Rossmeissl, (202) 586-8668; Materials & Electrochemical Research (MER) Corp. contact Dr. J. C. Withers, (520) 574-1980

Novel Catalyst for Carbon Monoxide Removal from Fuel Cell Reformate - DOE contact Ronald J. Fiskum, (202) 586-9154; KSE, Inc. contact Dr. James R. Kittrell, (413) 549-5506

A Fast, High Light Output Scintillator for Gamma Ray and Neutron Detection - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Radiation Monitoring Devices, Inc. contact Dr. Gerald Entine, (617) 926-1167

In-Situ Electron Beam Processing for Radio Frequency Cavities - DOE contact Jerry Peters, (301) 903-5228; FM Technologies, Inc. contact Dr. Frederick M. Mako, (703) 961-1051

An Innovative Fabrication Concept for Niobium-Tin Superconducting Wire - DOE contact Jerry Peters, (301) 903-5228; Alabama Cryogenic Engineering, Inc. contact Dr. John B. Hendricks, (256) 536-8629

High-Performance Niobium-Tin-Tantalum Superconductors Formed by Mechanical Alloying and Near-Net Shape Tube Filling - DOE contact Jerry Peters, (301) 903-5228; EURUS Technologies, Inc. contact John Romans, (850) 574-1800

INSTRUMENTATION AND FACILITIES

PHASE I

An Inexpensive, Efficient Neutron Monochromator - DOE contact Helen Kerch, (301) 903-2346; Adelphi Technology, Inc. contact Dr. Charles K. Gary, (650) 328-7337

High Performance Thermal Neutron Detector - DOE contact Helen Kerch, (301) 903-2346; Lexitek, Inc. contact Dr. Steven M. Ebstein, (781) 431-9604

Neutron and Electron Beam Instrumentation (MSC P1A20-205) - DOE contact Helen Kerch, (301) 903-2346; Materials Sciences Corporation contact Adam T. Rosen, (215) 542-8400

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 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 David Usher, (518) 464-3334

Four Probe Stage and Holder for Transmission Electron Microscope - DOE contact Dean Miller, (630) 252-4108; Zyvex Corporation contact Timothy M. Gilmoir, (972) 235-7881

INSTRUMENTATION AND FACILITIES

PHASE II (FIRST YEAR)

Sol-Gel Derived Neutron Detector Using a Lithiated Glass - DOE contact Helen Kerch, (301) 903-2346; Neutron Sciences, Inc. contact Andrew Stephan, (865) 523-0775

Development of an Ultra-Bright Electron Source for Scanning Transmission Electron Microscopy - DOE contact Dean Miller, (630) 252-4108; Nion Co. contact 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 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

PHASE I

LITS-Forming for Pre-Bending of Alumiunum Hydroformed Truck Frames - DOE contact Mike Kassner, (541) 737-7023; Native American Technologies Company contact Valerie L. Rhoades, (303) 279-7942

Development of a New, Low Frequency, Rf-Focused Linac Structure - DOE contact Jehanne Simon-Gillo, (301) 903-1455; Linac Systems contact Barbara C. Swenson, (505) 798-1904

SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE I

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

Insulation Coating of Rutherford Cable for Accelerator Applications - DOE contact Jerry Peters, (301) 903-3233; Global Research & Development, Inc. contact Michael Tomsic, (937) 332-0348

Fiber Optic Scintillator System for Detection of Beta Emitters in Groundwater - DOE contact Brendlyn Faison, (301) 903-0042; Adherent Technologies, Inc. contact Dr. Ronald E. Allred, (505) 346-1685

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

PHASE II (FIRST YEAR)

Advanced Membrane Technology for Biosolvents - DOE contact Charlie Russomanno, (202) 586-7543; Vertec Biosolvents, Inc. contact James E. Opre, (847) 803-0575

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE I

Hydroforming of Light Weight Components from Aluminum and Magnesium Sheet and Tube - DOE contact Mike Kassner, (541) 737-7023; Applied Engineering Solutions, LLC contact David Guza, (614) 789-9890

Carbon/Glass Hybrid Wind Turbine Blades - DOE contact John Cadogan, (202) 586-1991; ILT Corporation dba Think Composite contact Dr. Stephen W. Tsai, (650) 322-9433

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

PHASE II (FIRST YEAR)

Neutron Scattering Instrumentation for Measurement of Melt Structure - DOE contact Helen Kerch, (301) 903-2346; Containerless Research, Inc. contact John Nordine, (847) 467-2678

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE I

Waveshifters and Scintillators for Ionizing Radiation Detection - DOE contact Michael P. Procario, (301) 903-2890; Ludlum Measurements, Inc. contact Donald Ludlum, (915) 235-5494

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

PHASE II (FIRST YEAR)

Virtual-Impact Particle Sizing for Precursor Powders of Nb_3Sn and Bi-2212 Superconductors - DOE contact Jerry Peters, (301) 903-3233; Accelerator Technology Corporation contact Peter McIntyre, (979) 255-5531

Innovative Processing Methods for Superconducting Materials - DOE contact Jerry Peters, (301) 903-3233; Alabama Cryogenic Engineering, Inc. contact 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 Joseph Cheng, (937) 278-6547

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 micro structural 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 U.S., Japan, Europe, Russia, and China. The DOE contact is S. Berk (301) 903-4171.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

265. **VANADIUM ALLOY AND INSULATING COATING RESEARCH**
$2,000,000
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

266. **THEORY AND MODELING**
$1,200,000
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

267. **FERRITIC/MARTENSITIC STEEL RESEARCH**
$1,900,000
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

268. **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

269. **PLASMA FACING MATERIALS RESEARCH**
$1,800,000
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 ENVIRONMENTAL MANAGEMENT

	FY 2002
OFFICE OF ENVIRONMENTAL MANAGEMENT - GRAND TOTAL	$3,602,996
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,602,996
Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces	366,666
Radiation Effects on Sorption and Mobilization of Radionuclides During Transport Through the Geosphere	200,000
Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes	173,333
Radiation Effects in Nuclear Waste Materials	313,333
New Metal Niobate and Silicotitanate Ion Exchangers: Development and Characterization	300,000
Corrosion of Spent Nuclear Fuel: The Long-Term Assessment	148,333
Direct Investigations of the Immobilization of Radionuclides in the Alteration Products of Spent Nuclear Fuel	342,000
Physical, Chemical and Structural Evolutioon of Zeolite-Containing Waste Forms Produced from Metakaolinite and Calcined HLW	196,666
Investigating Ultrasonic Diffraction Grating Spectroscopy and Reflection Techniques for Characterizing Slurry Properties	229,333
Chemistry of Actinides in Molten Glasses and its Correlation to Structural Performance of Solid Glasses: Filling the Knowledge Gap	213,333
Stability of High Level Radioactive Waste Forms	286,666
Physical Characterization of Solid-Liquid Slurries at High Weight Fractions Utilizing Optical and Ultrasonic Methods	273,333
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 ENVIRONMENTAL MANAGEMENT

The Office of Environmental Management (EM) was established to effectively coordinate and manage the Department's activities to remediate the DOE Defense Complex and to properly manage waste generated by current operations. EM conducts materials research within two offices:

Office of Waste Management - The Office of Waste Management uses current technologies to minimize production of DOE-generated waste, alter current processes to reduce waste generation, and work with the Office of Science and Technology to develop innovative technologies for the treatment and disposal of present and future waste streams. The mission of the Office is to minimize, treat, store, and dispose of DOE waste to protect human health, safety, and the environment.

Office of Science and Technology - The Office of Science and Technology (OST) is responsible for managing and directing targeted basic research and focused, solution-oriented technology development programs to support the DOE Office of Environmental Management (EM). Programs involve research, development, demonstration, and deployment activities that are designed to produce innovative technologies and technology systems to meet national needs for regulatory compliance, lower life-cycle costs, and reduced risks to both people and the environment. Certain areas of the OST program focus on materials research in order to provide better, safer and less expensive approaches to identify, characterize and remediate DOE's waste problem.

Four Focus Areas have been formed to focus the EM-wide technology development activities on DOE's most pressing environmental management problems and are co-led by all EM offices:

Subsurface Contaminants. Hazardous and radioactive contaminants in soil and groundwater exist throughout the DOE complex, including radionuclides, heavy metals, and dense, nonaqueous phase liquids. Groundwater plumes have contaminated over 600 billion gallons of water and 50 million cubic meters of soil. In addition, the Subsurface Contaminants Focus Area is responsible for supplying technologies for the remediation of numerous landfills at DOE facilities. Technology developed within this speciality area provides effective methods to contain contaminant plumes and new or alternative technologies for remediating contaminated soils and groundwater.

Radioactive Tank Waste Remediation. Across the DOE Complex, hundreds of large storage tanks contain hundreds of thousands of cubic meters of high-level mixed waste. Primary areas of concern are deteriorating tank structures and consequent leakage of their contents. Research and technology development activities must focus on the development of safe, reliable, cost-effective methods of characterization, retrieval, treatment, and final disposal of the wastes.

Mixed Waste Characterization, Treatment, and Disposal. DOE faces major technical challenges in the management of low-level radioactive mixed waste. Several conflicting regulations together with a lack of definitive mixed waste treatment standards hamper mixed waste treatment and disposal. Disposal capacity for mixed waste is also expensive and severely limited. DOE now spends millions of dollars annually to store mixed waste because of the lack of accepted treatment technology and disposal capacity. In addition, currently available waste management practices require extensive, and hence costly waste characterization before disposal. Therefore, DOE must pursue technology that leads to better and less expensive characterization, retrieval, handling, treatment, and disposal of mixed waste.

Decontamination and Decommissioning. The aging of DOE's weapons facilities, along with the reduction in nuclear weapons production, has resulted in a need to transition, decommission, deactivate, and dispose of numerous facilities contaminated with radionuclides and hazardous materials. While building and scrap materials at the sites are a potential resource, with a significant economic value, current regulations lack clear release standards. This indirectly discourages the recovery, recycling, and/or reuse of these resources. The development of enhanced technologies for the decontamination of these materials, and effective communication of the low relative risks involved, will facilitate the recovery, recycle, and/or reuse of these resources. Improved materials removal, handling, and processing technologies will enhance worker safety and reduce cost.

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 EM's mission goals, and, in general, address problems that are considered intractable without new knowledge. This program is designed to inspire breakthroughs in areas critical to the EM mission through basic research and is managed in partnership with ER. ER's well-established procedures are used for merit review of applications to the EMSP. Subsequent to the formal scientific merit review, applications that are judged scientifically meritorious are evaluated by DOE for relevance to the objectives of the EMSP. The

FY 2002 EMSP portfolio consisted of approximately 200 awards amounting to a total of approximately $150 million in three-year funding. Fourteen of those awards were in scientific disciplines related to materials issues that have potential to solve Environmental Management challenges. The FY 2002 component of materials research is estimated to amount to $3,602,996. 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 EMSP Director for FY2002 was Mark Gilbertson. The current EMSP Director is Roland F. Hirsch (301) 903-9009.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

270. **ATMOSPHERIC-PRESSURE PLASMA CLEANING OF CONTAMINATED SURFACES**
$366,666
DOE Contact: Roland F. Hirsch (301) 903-9009
University of California at Los Angeles Contact: Robert F. Hicks (310) 206-6865
LANL Contact: Hans Herrmann (505) 665-6157

Decommissioning of transuranic waste (TRU) into low-level radioactive waste (LLW) represents the largest cleanup cost associated with the nuclear weapons complex. This project is developing a low-cost technology for converting TRU into LLW based on the selective plasma etching of plutonium and other actinides from contaminated structures. Plasma etching has already been used to remove Pu films from materials. However, this process is operated under vacuum, making it both expensive and difficult to apply to many nuclear wastes. A major breakthrough in this field was the demonstration of the operation of a g-mode, resonant-cavity, atmospheric-pressure plasma jet (APPJ). This jet etches kapton at between 10 and 15 m/hour, and tantalum at between 1 and 2 m/hour. Etching occurs below 373 K, so that delicate materials will not be destroyed by this process. The plasma jet may be used to selectively remove plutonium and other actinide elements by converting them into volatile compounds that are trapped by adsorption and filtration. Since the jet operates outside a chamber, many nuclear wastes may be treated, including machinery, duct-work, concrete and other building materials. At LANL, the source physics is being studied using Stark-broadening, microwave interferometry, and laser-induced fluorescence (LIF). The metastables, neutrals and radical species produced with mixtures of NF3, CF4, C2F6, O2,He and Ar are being identified by LIF, optical emission spectroscopy (OES), laser Raman spectroscopy (LRS), coherent anti-Stokes Raman spectroscopy (CARS), and mass spectroscopy (MS). At UCLA, the elementary surface reactions of these species with tantalum and tungsten (surrogate metals for Pu) are being studied in ultrahigh vacuum using a supersonic molecular-beam coupled to the plasma jet. The surfaces are being characterized by X-ray photoemission (XPS), infrared spectroscopy (IR), low-energy electron diffraction (LEED), and scanning-tunneling microscopy (STM). In addition, plutonium etching experiments are being carried out at the Los Alamos Plutonium Facility. Recent improvements in the source design have made it compact, rugged, reliable and easily configured to treat objects of different sizes and shapes. The objectives of this research program are to fully characterize the discharge physics and chemistry, to engineer the exhaust containment system, and to test the plasma device on contaminated structures within the Department of Energy complex.

Keywords: Plasma Etching, Plutonium

271. **RADIATION EFFECTS ON SORPTION AND MOBILIZATION OF RADIONUCLIDES DURING TRANSPORT THROUGH THE GEOSPHERE**
$200,000
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

272. **IRON PHOSPHATE GLASSES: AN ALTERNATIVE FOR VITRIFYING CERTAIN NUCLEAR WASTES**
$173,333
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

273. **RADIATION EFFECTS IN NUCLEAR WASTE MATERIALS**
$313,333
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

274. **NEW METAL NIOBATE AND SILICOTITANATE ION EXCHANGERS: DEVELOPMENT AND CHARACTERIZATION**
$300,000
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

275. **CORROSION OF SPENT NUCLEAR FUEL: THE LONG-TERM ASSESSMENT**
$148,333
DOE Contact: Roland F. Hirsch (301) 903-9009
University of Michigan Contact: Rodney C. Ewing (313) 647-8529

Spent nuclear fuel accounts for over 95% of the total radioactivity in the radioactive wastes in the United States that require disposal, disposition, or remediation. The UO_2 in spent nuclear fuel is not stable under oxidizing conditions. Under oxidizing conditions, the U(IV) has a strong tendency to exist as U(VI) in the uranyl molecule, UO_2^{2+}. The uranyl ions react with a wide variety of inorganic and organic anions to form complexes which are often highly soluble. The result is rather rapid dissolution of UO_2 and the formation of a wide variety of uranyl oxide hydrates, uranyl silicates and uranyl phosphates. The kinetics for this transformation are rapid, essentially instantaneous on geologic time scales. Under reducing conditions, UO_2 is stable, but may alter to U^{4+} compounds such as coffinite, $USiO_4$, depending on groundwater compositions. Under both oxidizing and reducing conditions, the formation of new uranium phases may lead to the release or retardation of trace elements, such as the fission product elements and actinides in spent nuclear fuel. Over the long term, and depending on the extent to which the secondary uranium phases can incorporate fission products and actinides, these alteration phases become the near-field source term.

Fortunately, previous experimental studies and field studies have established that natural uranite and its alteration products are good "natural analogues" for studying the corrosion of UO_2 in spent nuclear fuel. This research program is addressing the following issues:

1) What are the long-term corrosion products of natural UO_{2+x}, uraninite, under oxidizing and reducing conditions?

2) What is the paragenesis or the reaction path of the phases that form during alteration? How is the sequence formation related to the structure of these uranium phases and reacting groundwater composition?

3) What is the trace element content in the corrosion products as compared to the original UO_{2+x}? Do the trace element contents substantiate models developed to predict radionuclide incorporation into the secondary phases?

4) Are the corrosion products accurately predicted from geochemical codes (e.g., EQ3/6) that are used in performance assessments?

5) How persistent over time are the metastable phase assemblages that form? Will these phases serve as effective barriers to radionuclide release?

Experimental results and theoretical models for the corrosion of spent nuclear fuel under oxidizing and reducing conditions will be tested by comparison to results from studies of samples from the Oklo natural fission reactors.

Keywords: Uranium Oxides, Minerology, Corrosion, Phase Stability

276. **DIRECT INVESTIGATIONS OF THE IMMOBILIZATION OF RADIONUCLIDES IN THE ALTERATION PRODUCTS OF SPENT NUCLEAR FUEL**
$342,000
DOE Contact: Roland F. Hirsch (301) 903-9009
University of Notre Dame Contact: Peter C. Burns (219) 631-5380
Argonne National Laboratory Contact:
Dr. Robert J. Finch (630) 252-9829

This project emphasizes the synthesis of uranium phases and uranium phases doped with certain radionuclides in order to examine radionuclide incorporation in uranyl compounds. The identities of alteration phases important for spent-fuel corrosion will be gleaned from the results of long-term experiments on the corrosion of spent UO_2 fuel and unirradiated UO_2, as well as more recent studies of U-metal fuel corrosion, that are currently underway at ANL. The focus will be on synthesizing actinide compounds similar to those that have been identified as corrosion products of spent uranium-based fuels. The goals of the experiments are to synthesize and characterize actinide and fission-product host phases formed on U-based waste forms under oxidizing conditions, such as expected at the candidate geological repository at Yucca Mountain. Target phases for synthesis include those identified in current corrosion experiments with U-based fuels being conducted at Argonne. Those experiments demonstrate that many radionuclides are retained in U-bearing alteration products. Synthesis and characterization of U(VI) phases doped with specific radionuclides helps clarify the mechanisms of radionuclide incorporation into uranyl-based compounds. Where possible, stable-isotope equivalents of radionuclides are used during synthesis; however, pure Np and Pu analogues of selected uranium compounds will also be synthesized. In addition, U compounds doped with low levels of selected radionuclides will be characterized in order to understand mechanisms of trace-element substitution.
Methods used to characterize solid phases include X-ray powder diffraction and transmission electron microscopy. Selected samples are also analyzed by single-crystal X-ray structure analyses and X-ray absorption spectroscopy, where possible.

Keywords: Uranium Oxides, Minerology, Phase Stability, Corrosion, Radionuclides

277. **PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW**
$196,666
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

278. **INVESTIGATING ULTRASONIC DIFFRACTION GRATING SPECTROSCOPY AND REFLECTION TECHNIQUES FOR CHARACTERIZING SLURRY PROPERTIES**
$229,333
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

279. **CHEMISTRY OF ACTINIDES IN MOLTEN GLASSES AND ITS CORRELATION TO STRUCTURAL PERFORMANCE OF SOLID GLASSES: FILLING THE KNOWLEDGE GAP**
$213,333
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

280. **STABILITY OF HIGH LEVEL RADIOACTIVE WASTE FORMS**
$286,666
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

281. **PHYSICAL CHARACTERIZATION OF SOLID-LIQUID SLURRIES AT HIGH WEIGHT FRACTIONS UTILIZING OPTICAL AND ULTRASONIC METHODS**
$273,333
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

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

282. **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

283. **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 2002
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY - GRAND TOTAL	$12,730,821
OFFICE OF SPACE AND DEFENSE POWER SYSTEMS	$3,781,000
SPACE AND NATIONAL SECURITY PROGRAMS	$3,781,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,159,000
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	1,720,000
Carbon-Bonded Carbon Fiber Insulation Production, Maintenance, Manufacturing Process Development, and Product Characterization	439,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,622,000
Alloy Development Characterization, Mechanical Property Testing, and Insulation Outgassing Assessment	1,105,000
Fabrication Development and Materials Production for AMTEC Converters	517,000
OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION	$8,949,821
NUCLEAR ENERGY PLANT OPTIMIZATION	$3,555,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$3,555,000
Steam Generator Non-Destructive Examination Test Mockup Facility	260,000
Advanced Eddy-Current Inspection System for Detection and Characterization of Defects in Steam Generator Tubes	290,000
Develop Empirical Data to Characterize Aging Degradation of Polymers Used in Electrical Cable	330,000
Develop Condition Monitoring Techniques for Electrical Cable	270,000
Mechanical Behavior of Irradiated Structural Stainless Steels	465,000
Fatigue Management	400,000
Assessment of Aging Effects on Components and Structures from Nuclear Power Plants	500,000
Irradiation Induced Swelling and Stress Relaxation of PWR Reactor Core Internal Components	40,000
Mitigation of Initiation and Growth of PWSCC in Alloy 600 and 82/182 Weld Metals	125,000
Validation of BWR Fluence Models and Weldability of Internals	500,000
Low Temperature Hydrogen Cracking of Ni-base Alloys and Weld Metals	75,000
Master Curve Fracture Toughness Implementation	300,000
NUCLEAR ENERGY RESEARCH INITIATIVE	$4,569,821
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,863,089
Isomer Research: Energy Release Validation, Production and Applications	600,000
Incorporation of Integral Fuel Burnable Absorbers Boron and Gadolinium into Zirconium-Alloy Fuel Clad Material	321,342
Design of Radiation-Tolerant Structural Alloys for Generation IV Nuclear Energy Systems	641,875
Enhanced Thermal Conductivity Oxide Fuels	299,872

OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY (continued)

	FY 2002
NUCLEAR ENERGY RESEARCH INITIATIVE (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,706,732
Random Grain Boundary Network Connectivity as a Predictive Tool for Intergranular Stress-Corrosion Cracking	395,988
Fundamental Understanding of Crack Growth in Structural Components of Generation IV Supercritical Light Water Reactors	268,851
New Design Equations for Swelling and Irradiation Creep in Generation IV Reactors	458,552
Oxidation of Zircaloy Fuel Cladding in Water-Cooked Nuclear Reactors	206,209
Neutron and Beta/Gamma Radiolysis of Supercritical Water	477,403
Innovative Approach to Establish Root Causes for Cracking in Aggressive Reactor Environments	379,729
Improving the Integrity of Coated Fuel Particles: Measurements of Constituent Properties of SiC and ZrC, Effects of Irradiation, and Modeling	520,000
INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE	$825,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$825,000
Nano-Composited Steels for Nuclear Applications	475,000
Ex-Vessel Melt Coolability and Concrete Interaction during a Severe Accident (MCCI Project)	350,000

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

284. **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**
$1,720,000
DOE Contact: Robert Wiley (301) 903-2884
ORNL Contacts: J. Peyton Moore (865) 574-8258 and Evan Ohriner (865) 574-8519

Iridium alloy, DOP-26 (i.e., Ir-0.3 wt% W with Th and Al additions) is the fuel clad capsule material for radioisotope heat sources in space power systems for NASA missions. The production capabilities and facilities for producing blank and foil stock material at ORNL are maintained by continuing all production activities (powder processing, melting, extrusion, rolling, etc.) to supply limited quantities of blank and foil for clad vent set (CVS) production maintenance activities. The CVS production activity produces flight quality CVSs for inventory and maintains the production capabilities for future production campaigns. The iridium inventory for DOE is maintained, audited, and reported annually.

During FY 2002, 30 flight quality iridium alloy blanks and 0.3 square meters of foil were produced and stored. A commercial vendor was fully qualified for analysis of iridium alloys using glow discharge mass spectrometry. All approvals were obtained, and the vendor is being used routinely in this capacity. All documentation was obtained for five flight quality CVSs produced in FY 2001, and these were shipped to Los Alamos National Laboratory. Ten additional flight quality clad vent sets were produced and shipped.

Keywords: Iridium Processing, Melting Extrusion, Clad Vent Sets

285. **CARBON-BONDED CARBON FIBER INSULATION PRODUCTION, MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT, AND PRODUCT CHARACTERIZATION**
$439,000
DOE Contact: Robert Wiley (301) 903-2884
ORNL Contact: George Romanoski (865) 574-4838

CBCF type thermal insulation is employed in radioisotopic General Purpose Heat Source (GPHS) module assemblies for use in RPSs for space applications. This material was originally employed in GPHS-RTGs (Radioisotope Thermoelectric Generators) for Galileo/NASA (1989 launch) and Ulysses/NASA-European Space Agency (1990 lauch) missions. Material produced for the Cassini mission (1997 launch) was made with a replacement carbon fiber utilizing an optimized process and process controls. Several activities required for CBCF production and certification had not been exercised for a few years. When attempts were made to perform these activities, it was discovered that equipment and/or personnel changes had led to a loss of capabilities in some areas. The high-temperature vacuum furnace used for outgassing all test samples was rebuilt and requalified. Procedures for measuring ash content and thermal conductivity were rewritten and all approvals were obtained. It was discovered that at least one item of processing equipment was introducing impurities into the CBCF, and modifications or replacements were made as necessary.

Keywords: Insulation/Thermal, High Temperature Service, Carbon Fibers

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING

286. **ALLOY DEVELOPMENT CHARACTERIZATION, MECHANICAL PROPERTY TESTING, AND INSULATION OUTGASSING ASSESSMENT**
$1,105,000
DOE Contact: Robert Wiley (301) 903-2884
ORNL Contacts: Easo George (865) 574-5085,
J. Peyton Moore (865) 8258,
Robert Swindemann (865) 574-5108

This 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 and on the 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. Assessments are made of internal component materials for milliwatt generator outgassing characteristics.

Significant progress was made in several areas during FY 2002. Measurement of tensile properties on uniaxial samples of Haynes 25 were completed. These measurements include both base metal and weldment samples aged for up to 12,000 hours. Nine creep rupture tests and two creep rate tests were completed on Haynes 25. Results were within expectations for this alloy. Equipment was prepared for pressure burst testing of Haynes 25 capsules, and eight weld verification capsules were received from Los Alamos National Laboratory. Installation of these eight into testing facilities was initiated. A model was developed for the ductility of Haynes 25 as a function of exposure time at a temperature of 675 °C, and the influence of strain rate on ductility was measured. Final reports were prepared on grain growth in DOP-26 and DOP-40 iridium alloys. Attempts to define the influence of silicon on the properties of DOP-26 were unsuccessful because of problems with the production of suitable test alloys. A report was written on the insulator outgassing for the milliwatt generator, and tests were initiated to assess outgassing of an electrical heater that will be used for surrogate power in a sealed generator test.

Keywords: Iridium Alloys, Haynes 25, Material Characterization, Thermal Aging

287. **FABRICATION DEVELOPMENT AND MATERIALS PRODUCTION FOR AMTEC CONVERTERS**
$517,000
DOE Contact: Robert Wiley (301) 903-2884
ORNL Contacts: James King (865) 574-4807

The Advanced Radioisotope Power System (ARPS) Program has been developing AMTEC converters for power conversion in generators for NASA space missions. ORNL has contributed to this program in the areas of refractory metal alloy production, welding and brazing fabrication development and production of converters, measurement of total hemispherical emittance and thermal conductivity, magnetron sputtering of electrode coatings on Beta"-alumina tubes, and studies of oxidation kinetics.

In FY 2002, efforts continued to support the development of AMTEC cells. Additional arc-melted Mo-41%Re material was produced from powders, and plates and rods were supplied to Advanced Modular Power Systems, Inc. A promising alloy was identified for attaching Mo-41%Re to alumina insulators. This alloy has a melting temperature of 1170 °C, and compatibility testing indicated that it is unaffected by exposure to sodium.

Keywords: Molybdenum, Rhenium, Welding and Brazing, AMTEC

OFFICE OF TECHNOLOGY AND INTERNATIONAL COOPERATION

NUCLEAR ENERGY PLANT OPTIMIZATION

The Nuclear Energy Plant Optimization (NEPO) Program is a U.S. Department of Energy (DOE) Program research and development (R&D) program focused on the performance of currently operating U.S. nuclear power plants. The primary areas of focus for the R&D are plant aging and optimization of electrical production. Funding for the NEPO program comes from both the U.S. DOE and from private industry, with industry providing equal or greater matching funds for each NEPO project.

288. **STEAM GENERATOR (SG) NON-DESTRUCTIVE EXAMINATION (NDE) TEST MOCKUP FACILITY**
$260,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contact: J. Benson (650) 855-2146
ANL Contact: T. Wei (630) 252-4688

Task: Develop a library of well characterized, laboratory generated axial, circumferential, inner diameter and outer diameter cracks for use in assessing advanced NDE methods being developed by DOE and EPRI.

Results to Date:

- A glove box facility for NDE of tubes removed from service has been built.
- Inspection of six steam generator tube sections from the McGuire retired steam generators has been completed.
- A team of experts analyzed X-Probe data acquired from the steam generator mock-up.
- Inconel 600 tubing test samples containing stress corrosion cracks have been prepared.

Keywords: Stress Corrosion Cracking, Non-Destructive Examination, Steam Generator

289. **ADVANCED EDDY-CURRENT INSPECTION SYSTEM FOR DETECTION AND CHARACTERIZATION OF DEFECTS IN STEAM GENERATOR TUBES**
$290,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contact: J. Benson (650) 855-2146
ANL Contact: T. Wei (630) 252-4688

Task: Develop an advanced eddy-current inspection technique and data analysis methodology for more reliable detection and accurate sizing of defects in steam generator tubes.

Results to date:

- Bobbin and Motor-Driven Rotating Pancake Coil (MRPC) data has been acquired from a test section containing three axial cracks of varying depths. Data has been acquired with and without interfering artifacts, such as tube supports and deposits.
- An effort was initiated on the development of automated data analysis algorithms to perform the function of anomaly detection and classification.
- Work on developing software to automatically analyze eddy current data from array probes has begun.

Keywords: Stress Corrosion Cracking, Non-Destructive Examination, Steam Generator, Eddy-Current

290. **DEVELOP EMPIRICAL DATA TO CHARACTERIZE AGING DEGRADATION OF POLYMERS USED IN ELECTRICAL CABLE**
$330,000
DOE Contact: len W. Morris (301) 903-9527
EPRI Contact: G. Toman (704) 547-6073
SNL Contact: K. Gillen (505) 844-7494

Task: Compare natural aging to model predictions based on accelerated aging; obtain naturally-aged samples; develop and confirm aging models; investigate bonded jacket cable failure mechanisms; evaluate coaxial connector backshell moisture intrusion and moisture dams.

Results to date:

- Several cable aging methods have been developed which are expected to have significant impact to resolution of cable aging issues.
- First proof-of-principle experiments using the newly conceived wear-out approach show that it offers unique capabilities for predicting the remaining lifetimes of nuclear power plant cable materials.
- Bonded jacket insulation failure mechanism evaluation is complete. Two reports have been issued: “Investigation of Bonded Jacket Cable Insulation Failure Mechanisms” (1001002); “Investigation of Bonded Jacket Cable Insulation Failure Mechanisms: HELB Exposure Results” (1007635). The first report identified the aging fragility level for bonded jacket insulation with respect to LOCA functionality. The second test shows that even overaged cable does not crack in a HELB exposure.
- Coaxial moisture intrusion study is complete. The report “Evaluation of Moisture Intrusion into Coaxial Connectors” (1001390) has been issued.

Keywords: Polymers, Aging, Irradiation, Electrical Insulation

291. **DEVELOP CONDITION MONITORING (CM) TECHNIQUES FOR ELECTRICAL CABLE**
$270,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contact: G. Toman (704) 547-6073
SNL Contact: K. Gillen (505) 844-7494

Tasks: Activities under this project include the development of a basis with material-specific correlation between non-destructive examination (NDE) data and destructive examination for localized (sample) inspections. Other activities include development of electrical NDE techniques capable of detecting incipient defects along an entire cable run and NDE techniques suitable for implementation at nuclear power plants. In addition, the project will develop distributed fiber optic temperature/radiation sensing methodology.

Results to date:

- Early results show that two new conditions monitoring (CM) techniques based on modulus profiling and nuclear magnetic resonance measurements may be among the best CM techniques available for determining cable condition in existing nuclear power plants.

- Cable aging assessment training aids have been developed and are ready for use.
- A Beta version of the database software has been issued to DOE. Formal issuance of the database will occur in December 2002.
- The low-voltage compendium report was issued in January 2003.
- The medium voltage state of the industry report will be issued in mid-2003.

Keywords: Aging, Irradiation, Electrical Insulation, Fiber Optics, Condition Monitoring

292. **MECHANICAL BEHAVIOR OF IRRADIATED STRUCTURAL STAINLESS STEEL**
$465,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contact: H. T. Tang (650) 855-2012
ANL Contact: D. L. Porter (208) 533-7659

Tasks: The project will determine the mechanical behavior of irradiated structural stainless steels under conditions of interest to Light Water Reactors (LWR) and tools to predict component life. The project will also assess the results of NDE examinations and guide the timing of corrective actions. In addition, the project will determine the effect of irradiation history on the irradiation assisted stress corrosion behavior of multiple alloys of austenitic stainless steel and multiple heats of selected materials in Pressurized Water Reactor (PWR) water.

Results to date:

- In-cell constant extension-rate testing (CERT) system has been developed at ANL. This system is capable of simultaneous testing of two specimens in separate loading trains at different or identical displacement rates (10^{-2} to 10^{-8} inch/sec) and different or identical temperatures (up to 800 degrees Celsius). The system can be used for testing of various specimen designs, including tensile, fracture mechanics, and point-bend specimans.
- Mechanical testing performed showed saturation of tensile characteristics (yield stress, ultimate tensile strength, uniform elongation and total elongation) achieved at 5 to 15 dpa with saturation levels higher for the 316CW material than for 304SA material. All four (French and US) 316CW materials showed homogeneity of the mechanical characteristics after irradiation regardless of their initial characteristics and no grain size effect was noticed. Four 304L SA materials also showed homogeneous mechanical characteristics after irradiation.

Keywords: Austenitic Stainless Steel, Irradiation, Mechanical Properties, Modeling, Stress Corrosion Cracking

293. **FATIGUE MANAGEMENT**
$400,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contacts: J. Carey (650) 855-2105
S. Rosinski (704) 547-6123, B. Carter (704) 547-6019

Tasks: Provide cost-effective methods of evaluating the cyclic life of nuclear components, including the effects of reactor coolant environment. The methods will be based on the safety margins of the American Society of Mechanical Engineer (ASME) code. The project will also provide utilities with appropriate tools to manage fatigue effects.

Results to date:

- Issued an Interim Thermal Fatigue Guideline to assist utility operators in taking a proactive approach in preventing unplanned leakage from piping attached to reactor coolant systems.
- Developed an Interim model for a thermal fatigue screening tool.
- Issued draft Guidelines for Addressing Fatigue Environmental Effects for a Typical License Renewal Application. This document provides a method for considering reactor coolant environmental effects.

Keywords: Fatigue, ASME Code, Environmental Fatigue

294. **ASSESSMENT OF AGING EFFECTS ON COMPONENTS AND STRUCTURES FROM NUCLEAR POWER PLANTS**
$500,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contacts: J. Carey (650) 855-2105
S. Rosinski (704) 547-6123
ORNL Contact: T. M. Rosseel (865) 574-5380
PNNL Contact: S. K. Sundaram (509) 373-6665

Tasks: Obtain materials and components that have been in service in operating reactors to be used for comparison with laboratory aged materials to validate models for aging effects and non-destructive examination methods.

Results to date:

- The Big Rock Point Condition Assessment Project, which identified reactor and other plant components which would be acceptable candidates for future aging tests, is complete.
- A survey document has been prepared and disseminated to utility and other industry materials aging experts to identify key components which should be sampled for aging testing/model validation.
- Materials and specific sections of reactor vessel internals of decommissioned San Onofre Nuclear Generation Unit 1 (SONGS 1) have been identified for harvesting. Samples from baffle plate, former plate, and core barrel are being harvested.

Keywords: Aging, Non-Destructive Examinations, Modeling

295. **IRRADIATION INDUCED SWELLING AND STRESS RELAXATION OF PWR REACTOR CORE INTERNAL COMPONENTS**
$40,000
DOE Contact: Glen W. Morris (301) 903-9527
EPRI Contact: H. T. Tang (650) 855-2012

Tasks: Characterize irradiation-induced void swelling and stress relaxation related to degradation that could occur in operating reactors, and calibrate and extend the liquid metal reactor-based swelling model for PWR applications.

Results to date:

- A state-of-the-art review of void swelling and irradiation enhanced stress relaxation was performed. The review revealed small amounts of void swelling (0.1-0.5 percent) in baffle bolts removed from operating PWRs.
- To support the development of a method for in situ measurement of void swelling, tests were conducted using eddy current, Barkhausen noise, electro-potential and three ultrasonic (conventional, guided wave, and back-scattering) nondestructive techniques. The materials tested were sets of surrogate material with electrical resistivity and Young’s modulus altered by cold work or by use of powder metallurgy to determine the capability of each technique to measure 0.1 to 0.5% of void swelling. The eddy current, ultrasonic, and electro-potential methods have the most potential for field applications associated with the evaluation of void swelling and irradiation enhanced stress relaxation. These techniques will be used to evaluate void swelling attributes on irradiated materials, which represents a new application for these evaluation tools.

Keywords: Irradiation-Induced Swelling, Stress Relaxation

296. **MITIGATION OF INITIATION AND GROWTH OF PWSCC IN ALLOY 600 AND 82/182 WELD METALS**
$125,000
DOE Contact: Glen W. Morris (301) 903-9527

Task: The task will develop methodology to address the initiation and growth of primary water stress corrosion cracking in Alloy 600 and weld metals 182 and 82 for PWRs. This type of corrosion cracking has been identified in reactor pressure vessel welds for control rod drive mechanisms and in butt welds in 82 and 182 weld metal in a reactor vessel hot leg nozzle.

Results to date: In bid preparation stage.

Keywords: Stress Corrosion Cracking, Welds, PWR

297. **VALIDATION OF BWR FLUENCE MODELS AND WELDABILITY OF INTERNALS**
$500,000
DOE Contact: Glen W. Morris (301) 903-9527

Task: Material samples from BWR internal components will be obtained for use in benchmarking BWR fluence calculation methodologies and to provide additional data for determining weldability of BWR internal components.

Results to date: Contractors chosen; contracts being finalized.

Keywords: BWR, Welds, Fluence Calculation

298. **LOW TEMPERATURE HYDROGEN CRACKING OF Ni-BASED ALLOYS AND WELD METALS**
$75,000
DOE Contact: Glen W. Morris (301) 903-9527

Task: Hydrogen based cracking may occur rapidly at low temperatures. The task will evaluate if low temperature crack growth is significant for weld metal 182 in PWR service.

Results to date: Contractor chosen; contract being finalized.

Key Words: Hydrogen Cracking, Welds, PWR

299. **MASTER CURVE FRACTURE TOUGHNESS IMPLEMENTATION**
$300,000
DOE Contact: Glen W. Morris (301) 903-9527

Task: The existing reactor pressure vessel (RPV) codes, standards and regulations use highly conservative methods to determine the RPV material reference temperature. This task will provide the basis for establishing Master Curve fracture toughness methodology into codes, standards and regulations to allow excess conservatism to be removed from calculations to allow longer vessel life.

Results to date: Efforts to define and document appropriate margins for application of the Master Curve approach for RPV integrity assessment are underway. A process flow chart outlining the necessary variables has been generated.

Keywords: RPV, Master Curve, Fracture Toughness

NUCLEAR ENERGY RESEARCH INITIATIVE

Overall, the awarding of Nuclear Energy Research Initiative projects is expected to help preserve the nuclear science and engineering infrastructure within our Nation's universities, laboratories and industries, as well as advance the state of nuclear energy technology and to maintain a worldwide competitive position. In regard to materials research, Nuclear Energy Research Initiative projects are performed in order to address issues related to the design and development of advanced nuclear reactors or to understand materials phenomena in existing reactors.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

300. **ISOMER RESEARCH: ENERGY RELEASE VALIDATION, PRODUCTION AND APPLICATIONS**
$600,000
DOE Contact: C. Thompson (301) 903-3918
LLNL Contact: J. A. Becker (925) 422-9676

The goal of this applied nuclear isomer research program is the search for, discovery of, and practical application of a new type of high energy density material (HEDM). Nuclear isomers could yield an energy source with a specific energy as much as a hundred thousand times as great as that of chemical fuels. There would be enormous payoffs to the Department of Energy and the country as a whole if such energy sources could be identified and applied to a range of civilian applications.

Despite the potential payoff, efforts in applied isomer research have been rather limited and sporadic. There has been basic research on nuclear isomers since their discovery in 1935 with an occasional hint to tantalize interest in HEDM. In most cases, these hints were refuted by careful examination by other groups.

The isomer area is rich with possibilities. We have prioritized several areas likely to be the most rewarding and fruitful for initial experimental and theoretical investigation because these areas directly bear on important issues, such as the following:

- Can the energy stored in nuclear isomers be released on demand?
- Is the size of the atomic-nuclear mixing matrix element large enough to be useful?
- Can we initiate quantal collective release of isomeric energy from a crystal?
- What is the precise energy of the 3.5 eV level in ^{229m}Th?

The specific target experiments are:

- X-ray induced decay of ^{178m2}Hf with a sensitivity 10^5 times recent work
- NEET: A measurement of the atomic-nuclear mixing matrix element in ^{189}Os
- Superradiance in ^{93m}Nb
- TEEN: Nuclear isomer energy release in ^{178m2}Hf
- Energy and lifetime of the ^{229m}Th isomeric level at 3.5 eV

Keywords: Isomer, NEET, TEEN, HEDM, High Energy Density Material

301. **INCORPORATION OF INTEGRAL FUEL BURNABLE ABSORBERS BORON AND GADOLINIUM INTO ZIRCONIUM-ALLOY FUEL CLAD MATERIAL**
$321,342
DOE Contact: C. Thompson (301) 903-3918
University of Wisconsin Contact: K. Sridharan (608) 263-4789

Long-lived fuels require the use of higher enrichments of U-235 or other fissile materials. Such high levels of fissile material lead to excessive fuel activity at the beginning of life. To counteract this excessive activity, integral fuel burnable absorbers (IFBA) are added to some rods in the fuel assembly. The three commonly used IFBA absorbers are gadolinium oxide and erbium oxide which are added to the UO_2 powder, and zirconium-diboride which is applied as a coating on the UO_2 pellets using plasma spraying or chemical vapor deposition techniques. These operations are performed as part o the fuel manufacturing process in the fuel plants. due to the potential for cross-contamination with fuel that does not contain IFBA, these operations are performed in a facility that is physically separated from the main plant. These operations tend to be very costly because of their small volume and can add from 20 to 30% to the manufacturing cost of the fuel. Other manufacturing issues that impact cost are maintaining the correct levels of dosing and the reduction in fuel melting point due to gadolinium and erbiuim oxide additions.

The goal of the proposed research is to develop an alternative approach that involves incorporation of boron or gadolinium into the fuel cladding material rather than as a coating or additive to the fuel pellets. This paradigm shift will allow for the introduction of the IFBA in a non-nuclear regulated environment and will obviate the necessity of additional handling and processing of the fuel pellets. This could represent significant cost savings and potentially lead to greater reproducibility and control of the burnable fuel in the early stages of the reactor operation.

We propose the use of state-of-the-art ion-based surface engineering techniques to achieve this objective. Specifically, we propose the application of IBEST (Ion Beam Surface Treatment) process being developed at Sandia National Laboratory, which involves the delivery of high-energy ion beam pulses onto the surface of a target material. These pulses melt the top few microns of the target material's surface. The melt zone then solidifies rapidly at rates in excess of 10^9 K/sec due to rapid heat extraction by the underlying substrate heat sink. This rapid solidification allows for surface alloying well in excess of the thermodynamically dictated solubility limits. This effect can be beneficially applied to the objectives of the proposed research for incorporating boron or gadolinium into the near-surface regions of Zircaloy-4 and Zirlo material used for fuel cladding. Several variants of this approach will be investigated with the goal of optimizing the process parameters to achieve the desired structure, composition, and compositional gradiant in the near-surface regions of the Zircaloy-4 and Zirlo that, in addition to the incorporation of boron or gadolinium into the surface, also yield improvements in surface hardness and oxidation resistance.

Keywords: Boron, Gadolinium, Erbium, IBEST, Ion Beam Surface Treatment, IFBA, Integral Fuel Burnable Absorbers, Nuclear Fuel Development

302. **DESIGN OF RADIATION-TOLERANT STRUCTURAL ALLOYS FOR GENERATION IV NUCLEAR ENERGY SYSTEMS**
$641,875
DOE Contact: C. Thompson (301) 903-3918
ANL Contact: T. Allen (208) 533-7760

The irradiation performance of structural materials will likely be the limiting factor in successful nuclear energy system development. The limits of the structural and fuel materials determine the performance of new nuclear energy systems. Satisfactory performance in a nuclear energy system is unusually demanding. In addition to the best characteristics and performance of materials that have been achieved in other advanced high temperature energy systems, nuclear energy systems require exceptional performance under high fluence irradiation. Based on experience, materials not tailored for irradiation performance generally experience profound changes in virtually all important engineering and physical properties because of fundamental changes in structure caused by radiation damage.

This project will develop and characterize the radiation performance of materials with improved radiation resistance. Material classes will be chosen that are expected to be critical in multiple Generation IV technologies. The material design strategies to be tested fall into three main categories: 1) alloying, by adding oversized elements to the matrix; 2) engineering grain boundaries; and 3) microstructural/nanostructural design, such as adding matrix precipitates.

The materials to be examined include both austenitic and ferritic-martensitic steels, both classes of which are expected to be key structural materials in many Generation IV concepts. The irradiation program will consist of scoping studies using proton and heavy-ion irradiations of key alloys and tailored alloy conditioning and examination of materials irradiated in BOR-60 to confirm charged particle results. Examinations will include microstructural characterization, mechanical properties evaluation using hardness and shear punch, and stress corrosion cracking.

Keywords: BOR-60, Irradiation, Microstructural, Nanonstructural, Nuclear

303. **ENHANCE THERMAL CONDUCTIVITY OXIDE FUELS**
$299,872
DOE Contact: C. Thompson (301) 903-3918
Purdue University Contact: A. A. Solomon (765) 494-5753

The objective of the proposed research is to produce a novel oxide fuel form with superior thermal conductivity. The resulting fuel will be applicable to existing light-water reactors, especially with high burn-up, high-performance fuels. It is also expected that such fuel will provide superior performance in advanced reactors that would otherwise be fueled with low-conductivity oxide fuels.

Keywords: Oxide Fuels, Light Water Reactor, Thermal Conductivity

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

304. **RANDOM GRAIN BOUNDARY NETWORK CONNECTIVITY AS A PREDICTIVE TOOL FOR INTERGRANULAR STRESS-CORROSION CRACKING**
$395,988
DOE Contact: C. Thompson (301) 903-3918
LLNL Contact: W. King, (925) 423-6547

In this work, we will develop methods to quantify the interconnectivity of the random grain boundary network, measure the interconnectivity of a series of materials where the interconnectivity has been systematically altered. We then perform property measurements on the materials and compare their performance ranking with the boundary network measurements, and characterize the materials to correlate actual crack paths with the measurements of the random grain boundary network.

With this data, we will then evaluate and improve the methods that have been chosen to describe the random grain boundary network. We will test the characterization method by evaluating the interconnectivity of the random grain boundary network in a series of as-received materials, rank their expected performance, and compare the results with property measurements.

The major accomplishments of this project are expected to be 1) the determination that the random boundary network connectivity (RBNC) is a major driver of IGSCC in low to medium stacking fault energy austenitic alloys, 2) the development of a predictive tool for ranking IGSCC performance of these alloys, and 3) the establishment of thermochemical processing parameters to be applied in the manufacture of IGSCC resistant materials. The outcome of the project will be identification of a mitigation strategy for IGSCC in current LWR conditions that can then enable the development of economically and operationally competitive water-cooled advanced reactor systems.

Keywords: Random Grain Boundary Network, RBNC, Intergranular Stress Corrosion Cracking

305. **FUNDAMENTAL UNDERSTANDING OF CRACK GROWTH IN STRUCTURAL COMPONENTS OF GENERATION IV SUPERCRITICAL LIGHT WATER REACTORS**
$268,851
DOE Contact: C. Thompson (301) 903-3918
SRI International Contact: I. Balachov (650) 859-3238

This work will contribute to the design of safe and economical Generation IV Supercritical Light Water Reactors (SCLWR) by providing a basis for selecting structural materials to ensure functionality of in-vessel components during the entire service life and estimating the lifetime of structural components under a variety of normal and offset operation conditions.

The objectives of this project are:

- Increase understanding of the fundamentals of crack growth in structural components of Generation IV SCLWR made of stainless steels and nickel-based alloys at supercritical temperatures.
- Provide tools for assessing the influence of the operating conditions in power plants with supercritical coolant temperatures on the electrochemistry of different types of corrosion processes taking place in the coolant circuits of supercritical power plants.
- Measure material-specific parameters describing the material's susceptibility to stress corrosion cracking and other forms of environmentally assisted degradation of structural materials at supercritical coolant conditions.
- Use these measurements to interpret the rate-limiting processes in the corrosion phenomena and as input data for lifetime analysis.
- Use the SRI-developed FRASTA (Fracture surface topography analysis) technique to obtain information on crack nucleation times and crack growth rates via analysis of conjugate fracture surfaces. Identify candidate remedial actions by which the susceptibility to stress corrosion cracking can be decreased

A unique combination of two advanced techniques for studying material reliability will be used. Controlled Distance Electrochemistry (CDE) will allow us to determine in relatively short experiments a measurable material parameter that describes the transport of ions or ionic defects in the oxide films and that will be correlated with the susceptibility to cracking, using fracture surface topography analysis (FRASTA) to reconstruct the evolution of crack initiation and growth.

Keywords: Crack Growth, Corrosion, Fracture Surface Topography Analysis, Controlled Distance Electrochemistry

306. **NEW DESIGN EQUATIONS FOR SWELLING AND IRRADIATION CREEP IN GENERATION IV REACTORS**
$458,552
DOE Contact: C. Thompson (301) 903-3918
LLNL Contact: W. G. Wolfer (925) 423-1501

Our understanding of void swelling and irradiation creep has been challenged recently by new discoveries that necessitate the development of a more comprehensive modeling of microstructural evolution under irradiation, and a derivation of new constitutive equations for swelling and irradiation creep different from those in the past. The microstructural foundations of these new constitutive laws will provide design equations for swelling and irradiation creep which can be confidently extrapolated and applied to Generation IV reactor concepts. Some of these new discoveries include the commencement of void swelling at lower doses with lower dose rates; the occurrence of void swelling in LWRs and at temperatures lower than previously believed possible; the observations of high concentrations of hydrogen in LWR components which exhibit void swelling, implicating hydrogen in addition to helium as a nucleating agent for voids; and the finding that irradiation creep is first enhanced when void swelling commences, but then declines and nearly vanishes as a steady-state swelling rate is approached. These new discoveries are the result of having constructed and analyzed an extensive database from many different irradiation experiments. The proposed comprehensive modeling of void nucleation and evolution of the microstructure is now made possible with the dramatic advancements in scientific computing afforded by the ASCI (Advanced Strategic Computing Initiative).

We are proposing to develop the theoretical models and the computer simulation codes to predict the evolution of the microstructure in structural materials exposed to neutron irradiations and to the chemical and thermo-mechanical environments in Generation IV reactors as well as existing reactors. In addition, we propose to develop also compact, macroscopic constitutive equations for swelling and irradiation creep that can be used in reactor design and performance evaluation.

We are pursuing a dual approach in this project, which consists of two coupled feedback loops of model development and model verification. One feedback loop encompasses the microstructural models and TEM data from irradiated samples. The other feedback loop deals with macroscopic constitutive laws for swelling and irradiation creep and their calibration with data from density measurements and creep strains. The two loops are connected by the derivation of the functional form of the constitutive laws from the microstructural models. The duel validation at the microscopic and the macroscopic level will greatly enhance the consistency and the validity of the predictions when the performance parameters of Generation IV reactors are outside the range for existing reactors.

Keywords: Microstructure, Macrostructure, Void Swelling, Irradiation Creep, Generation IV, LWR

307. **OXIDATION OF ZIRCALOY FUEL CLADDING IN WATER-COOKED NUCLEAR REACTORS**
$206,209
DOE Contact: C. Thompson (301) 903-3918
Pennsylvania State University Contact:
D. MacDonald (814) 863-7772

With the development of higher burn-up fuels for nuclear power reactors, much greater demands are being placed on the performance of the Zircaloy fuel sheaths. The principle threat to the integrity of the sheath is oxidation/corrosion and hydriding, leading to more-or-less uniform thinning and, in some instances, to localized corrosion in the form of nodular attack and/or hydriding. Failure leads to the release of fission products into the coolant, which in turn contributes to the man-REM costs of operating the system. Extensive fuel failures may require shutdown, which results in the unit being unavailable for normal operation. Thus, strong operational and economic reasons exist for enhancing fuel reliability. The principle goal of the proposed work is to develop sophisticated physico-electrochemical models for the corrosion of Zircaloy fuel sheaths that can be used by reactor operators to *actively manage* the accumulation of damage and hence to minimize the risk of fuel cladding failure in operating reactors.

The proposed research will represent a *major* departure from work being carried out elsewhere, in that it will:

- Incorporate the Point Defect Model (PDM) in place of the diffusion models to describe oxide *and hydride* growth.
- Incorporate the cathodic reactions that occur at the fuel caldding/coolant interfacing including the role of intermetallic precipitates in the film as catalytic sites for these reactions.
- Incorporate an advanced coolant radiolysis model for estimating the concentrations of electroactive species (oxygen, hydrogen peroxide, hydrogen, etc.) at the cladding surface, as a function of the chemistry of the coolant (pH, [Li], [B], [H_2]) and the operating conditions of the reactor.
- Include the mechanisms (cation vacancy condensation) for passivity breakdown as a means of describing the onset of nodular attack.
- Develop a model based upon the generation and annihilation of point defects (oxygen vacancies, cation vacancies, and zirconium interstitials) at the Zircaloy/zirconia and zirconia/solution interfaces to describe the generation of stress in the interphasial region.
- Incorporate a model for the concentration of solutes into porous deposits (CRUD) on the fuel under boiling (BWRs) or nucleate boiling (PWRs) conditions, in order to more accurately describe the environment that is in contact with the Zircaloy surface.

- Integrate the damage over the operating history of the reactor, including start-ups, shut downs, and variable power operation.
- Explore the electronic structure and measure kinetic parameters for ZrO_2 film growth on Zircaloy under accurately simulated reactor operating conditions. Film growth will be followed *in situ* by electrochemical impedence spectroscopy (EIS)/capacitance measurements, whereas the electronic structure will be determined by using Mott-Schottky analysis.
- Measure kinetic parameters (exchange current densities and transfer coefficients) for the reduction of oxygen and the oxidation of hydrogen on Zircaloy under prototypical reactor operating conditions, these data being required to accurately model the cathodic processes that occur on the cladding surface.

The output of this project will be a more comprehensive understanding of the oxidation and hydriding of Zircaloy fuel cladding in reactor coolant environments, with particular emphasis on linkage between the plant operating parameters and the damage incurred due to oxidation and hydriding. Additionally, the project will yield a set of models and codes that will be made available to the nuclear power industry for managing the accumulation of corrosion damage to reactor fuel cladding as a function of the coolant chemistry and reactor operating conditions and history.

Finally, the development of the models and codes outlined in this proposal could greatly aid in the development of Generation IV reactors, by exploring water chemistry, materials/environment compatibility, and fuel design options that would minimize corrosion (oxidation and hydriding) damage to fuel cladding under specified operating regimes.

Keywords: Electrochemical Impedence Spectroscopy, EIS, Hydriding, Zircaloy, Oxidation, Corrosion, Point Model Defect, PMD

308. **NEUTRON AND BETA/GAMMA RADIOLYSIS OF SUPERCRITICAL WATER**
$477,403
DOE Contact: C. Thompson (301) 903-3918
ANL Contact: D. M. Bartels (630) 252-3485

Commercial nuclear reactors provide a source of heat, used to drive a “heat engine” (turbine) to create electricity. A fundamental result of Thermodynamics shows that the higher the temperature at which any heat engine is operated, the greater its efficiency. Consequently, one obvious way to increase the operating efficiency and profitability for future nuclear power plants is to heat the water of the primary cooling loop to higher temperatures. Current pressurized water reactors run at roughly 300 °C and 100 atm pressure. Designs under consideration would operate at 450 °C and 250 atm, i.e., well beyond the critical point of water. This would improve the thermodynamic efficiency by about 30%. The major unanswered questions are: What changes will occur in the radiation-induced chemistry in water as the temperature and pressure are raised beyond the critical point, and what does this imply for the limiting corrosion processes in the materials of the primary cooling loop?

The cooling water of any water-cooled reactor undergoes radiolytic decomposition, induced by gamma, fast-electron and neutron radiation in the reactor cores. Unless mitigating steps are taken, oxidizing species produced by the coolant radiolysis can promote intergranular stress-corrosion cracking and irradiation-assisted stress-corrosion cracking of iron- and nickel-based alloys. These will alter corrosion rates of iron- and nickel-based alloys, and zirconium alloys in reactors. One commonly used remedial measure to limit corrosion by oxidizing species is to add hydrogen in sufficient quantity to chemically reduce transient radiolytic primary oxidizing species (OH, H_2O_2, H_2O/O_2), thereby stopping the formation of oxidizing products (H_2O_2 and O_2). It is still unclear whether this will be effective at the higher temperatures proposed for future reactors. While an earlier NERI project has investigated some of the most important radiation chemistry in supercritical water, there is no information at all on the effect of neutron radiolysis, which is the main source of the troublesome oxidizing species.

The collaboration proposed here is ideally suited to discover most of the fundamental information necessary for a predictive model of radiation-induced chemistry in a supercritical water reactor core. Electron pulse radiolysis coupled with transient absorption spectroscopy is the method of choice for measuring kinetics of radiation-induced species, and also product yields for fast electron and gamma radiation. The Argonne Chemistry Division linac is capable of producing 20 MeV electron pulses of 30 picoseconds duration, and the principal investigators at Argonne have extensive experience in measuring transients on a nanosecond and sub-nanosecond timescale. The University of Wisconsin Nuclear Reactor Facility is a very convenient source of neutron radiation that can be exploited for radiolysis experiments from room temperature to 500°C. The combined capabilities will make it possible to create a quantitative model for water radiolysis in both current PWR systems and supercritical water-cooled plants in the future.

Keywords: Radiolysis, Radiolytic Decomposition, Supercritical Water, Intergranular Stress Corrosion Cracking, IGSCC

309. **INNOVATIVE APPROACH TO ESTABLISH ROOT CAUSES FOR CRACKING IN AGGRESSIVE REACTOR ENVIRONMENTS**
$379,729
DOE Contact: C. Thompson (301) 903-3918
PNNL Contact: S. M. Bruemmer, (888) 375-7665

The successful development of Generation IV nuclear power systems must address and mitigate several materials degradation issues now strongly impacting existing light water reactors (LWRs) after very long periods of operation. In addition, the more aggressive radiation and environmental exposures envisioned for various advanced reactor concepts will require materials with improved high-temperature properties and resistance to cracking. Although previous fast reactor and fusion device programs have focused on the development of improved structural materials for their relevant conditions, no comparable effort has been directed toward the conditions unique to water-cooled fission reactors since the inception of nuclear-powered propulsion units for submarines. The paramount issue impacting both LWR economics and safety has been corrosion and stress corrosion cracking in high-temperature water. These degradation processes have continued to limit performance as the industry has changed operating parameters and materials. Mechanistic understanding and non-traditional approaches are necessary to create durable corrosion-resistant alloys and establish the foundation for advanced reactor designs. Less down time and longer component lifetimes are the drivers motivating this research for both Generation III and IV nuclear-power systems.

Proposed research will focus on the characterization of critical Fe- and Ni-based stainless alloys tested under well-controlled conditions where in-service complexities can be minimized. Quantitative assessment of crack-growth rates will be used to isolate effects of key variables, while high-resolution analytical transmission electron microscopy will provide mechanistic insights by interrogating crack-tip corrosion/oxidation reactions and crack-tip structures at near atomic dimensions. Reactions at buried interfaces, not accessible by conventional approaches, will be systematically interrogated for the first time. Novel mechanistic “fingerprinting” of crack-tip structures tied to thermodynamic and kinetic modeling of crack-tip processes will be used to isolate causes of environmental cracking. Comparisons will be made with results on failed components removed from LWR service (funded separately by industry collaborators).

The proposed research strategy capitalizes on unique national laboratory, industry and university capabilities to generate basic materials and corrosion science results with immediate impact to next-generation nuclear power systems. This proposed work will be integrated with existing NERI projects, with fundamental research funded by the DOE Office of Basic Energy Sciences and with focused U.S. and international projects dealing with current LWR degradation issues. This leveraged approach will facilitate the revolutionary advances envisioned in NERI by creating a multi-faceted effort combining the basic and applied science necessary to drive mechanistic understanding and promote development of next-generation materials that meet advanced reactor performance goals.

Keywords: Crack-Tip, Advanced Nuclear Reactor, LWR, Stress Corrosion, Crack Growth

310. **IMPROVING THE INTEGRITY OF COATED FUEL PARTICLES: MEASUREMENTS OF CONSTITUENT PROPERTIES OF SiC AND ZrC, EFFECTS OF RADIATION, AND MODELLING**
$520,000
DOE Contact: C. Thompson (301) 903-3918
ORNL Contact: L. L. Snead (865) 574-9942

The SiC layer integrity in the TRISO-coated gas-reactor fuel particle is critical to the performance, allowed burn-up, hence intrinsic efficiency of high temperature gas-cooled reactors. While there has been significant developmental work on manufacturing the fuel particles, detailed understanding of what effects the complex in-service stress state combined with realistic materials property data under irradiation has on fuel particle survival is not adequately understood. Furthermore, zirconium carbide, which has been proposed as a higher-temperature replacement for SiC, has virtually no experimental database on the effects of irradiation on thermo-mechanical properties. The basic assertion behind this proposal is that significant need exists for detailed fuel particle modeling including realistic, experimentally derived data on fuel particle constituent materials in the non-irradiated and irradiated condition. To perform this work will require advances in modeling, along with technique development for measurement of materials properties at the small scale of the fuel particle.

Proposed elements of work:

<u>Modeling Work.</u> In recent years, a collaboration has been established between INEEL and MIT looking into finite element and other methods of modeling the stress state of fuel pellets. This has been carried to the point where it is being limited by the lack of realistic material property input. Specific input on SiC statistical distribution of strength, creep and swelling are poorly described in the literature. Thermo-mechanical properties of pyrolytic ZrC are also very limited. These new data will be generated and applied in model spherical and cylindrical geometry. The objective of this work is to use the new data to better describe the stress state of the TRISO particle under irradiation and to give a direct comparison of the integrity

of SiC-v-ZrC for this application. Potential failure during pellet processing will also be addressed.

Technique Development for Measurement of Constituent Properties. To this point, techniques to study the integrity of fuel particles have been relatively rudimentary, consisting of compression tests (crush or c-ring) of the particle or bare SiC overcoat. The objective of this element is to apply state-of-the-art techniques and to develop new techniques specifically for application to the TRISO system to generate realistic data for the modeling. These techniques would then become available for the gas-cooled reactor fuels development community. Specific tools will be developed to measure strength through internal pressurization, elastic modulus on the scale of the TRISO particle, creep relaxation, and PyC/SiC interfacial properties.

Irradiation Materials Property Information. An irradiation program will be coupled with the technique development program to generate mechanical property information needed for modeling input. Irradiation program will include model, non-fueled cylindrical and spherical TRISO structures, and spherical TRISO containing helium producing boron carbide.

Updated Materials Data Handbook for TRISO fuels. As part of this effort, a materials property handbook will be developed. This handbook will include pertinent physical property information on all constituent materials of coated particle fuel. Sources of information will be both taken from the open nuclear materials literature, reports dealing with HTGR's (e.g., CEGA-002820, Rev 1), and information developed as part of this proposal. This material will then be available to the larger fuels community.

Keywords: TRISO, SiC, Fuel Particles, Irradiation

INTERNATIONAL NUCLEAR ENERGY RESEARCH INITIATIVE

The I-NERI sponsors innovative scientific and engineering R&D, in bilateral cooperation with participating countries, to address the key issues affecting the future of nuclear energy and its global deployment. The goal of I-NERI is to develop advanced technologies to improve cost performance, enhance safety, and increase proliferation resistance of future nuclear energy systems. The primary objectives of the I-NERI Program in accomplishing this goal are to:

- Develop advanced concepts and scientific breakthroughs in nuclear energy and reactor technology to address and overcome the principal technical and scientific obstacles to the expanded use of nuclear energy worldwide
- Promote bilateral collaboration with international agencies and research organizations to improve development of nuclear energy
- Promote and maintain the nuclear science and engineering infrastructure to meet future technical challenges

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

311. **NANO-COMPOSITED STEELS FOR NUCLEAR APPLICATIONS**
$475,000
DOE Contact: S. Schuppner (301) 903-1652
ORNL Contact: Roger E. Stoller (865) 576-7886

The successful development of advanced nuclear technologies embodied in the overall concept of Generation IV reactors will provide major challenges to the field of materials science. An underlying theme common to all systems under consideration is the critical importance of developing fuel cladding and structural materials that outperform the best of the materials currently code-qualified for in-core applications. For example, the development of alloys with greatly improved creep strength, fracture resistance, and oxidation resistance combined with a high degree of tolerance for radiation damage would enable systems to be designed with higher operating temperatures and extended component lifetimes.

Alloy development efforts in Japan, Europe, and the U.S. have shown that nano-composited versions of the $Fe^{-8}Cr$ ferritic-martensitic and $Fe^{-13}Cr$ ferritic steels have the potential for developing into a new class of creep- and oxidation-resistant steels with outstanding swelling resistance that could be deployed in Generation IV reactor systems. Work is continuing at various institutions to address issues such as anisotropic properties, thermal embrittlement, strength loss associated with microstructural instabilities, and compatibility with liquid and gaseous environments.

This collaborative proposal seeks to develop a scientific knowledge base on the fundamental deformation and fracture characteristics of several carefully selected representative nano-composited steels strengthened by fine scale oxide particles or atom clusters rich in yttria, titanium, and oxygen. This information will be combined with a study of the effects of neutron irradiation on microstructural stability and mechanical behavior to provide a solid foundation for further development of these innovative materials for nuclear applications.

Miniaturized tensile, creep, and fracture testing techniques will be used, coupled with microstructural characterization to define a limited set of promising composition/microstructures for neutron irradiation studies. Nano-scale structural characterization will be carried out to provide input to microstructure-property modeling activities. Extensive use of Ashby deformation and fracture mapping will be made to characterize the dominent regimes of deformation and fracture processes. A preliminary assessment will be made of the radiation response of a limited number of promising composition/microstructures; irradiations will be carried out using experimental facilities at Phenix, HFIR, or JOYO. The impact of neutron irradiation on the deformation and fracture regimes will be mapped. Relationships between the radiation-modified microstructure and the dominant modes of deformation and fracture will be modeled. This information will be integrated with that obtained from other programs to develop a thorough evaluation of the potential of these materials for expanding the operating temperature limits of fission reactor systems.

Keywords: Microstructure, Irradiation, Ferritic, Martensitic, Steel, Embrittlement

312. **EX-VESSEL MELT COOLABILITY AND CONCRETE INTERACTION DURING A SEVERE ACCIDENT (MCCI PROJECT)**
$350,000
DOE Contact: S. Schuppner (301) 903-1652
ANL Contacts: J. L. Binder (630) 252-7265 and M. T. Farmer (630) 252-4539

The MCCI program is a collaborative project between the Reactor Analysis and Engineering (RAE) Division of Argonne National Laboratory, the U.S. Nuclear Regulatory Commission, and a consortium of ten international participants represented by the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development. U.S. NRC is the Operating Agent for the program.

Although extensive research has been conducted over the last several years in the areas of melt coolability and core-concrete interaction, two important issues warrant further investigation. The first issue concerns the effectiveness of water in terminating a core-concrete interaction by flooding the interacting masses from above, thereby affecting a quench of the molten core debris and rendering it permanently coolable. The second issue concerns long-term two-dimensional ablation by a prototypic core oxide melt. The goal of the MCCI research program is to conduct reactor material experiments and associated analysis to achieve the following two technical objectives: 1) Resolution of the ex-vessel debris coolability issue through a program which focuses on providing both confirmatory evidence and test data for the coolability mechanisms identified in MACE integral effects tests; and 2) Address remaining uncertainties related to long-term two-dimensional core-concrete interaction under both wet and dry cavity conditions. Achievement of these two main objectives will lead to improved accident management guidelines for existing plants and also better containment designs for future plants.

Keywords: Melt Coolability, Core-Concrete Interaction

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2002
NATIONAL NUCLEAR SECURITY ADMINISTRATION - GRAND TOTAL	$114,492,000
OFFICE OF NAVAL REACTORS	$79,200,000[1]
OFFICE OF DEFENSE PROGRAMS	**$**20,069,000
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM	**$**20,069,000
SANDIA NATIONAL LABORATORIES	$14,486,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$6,054,000
Materials Synthesis	1,042,000
Metal Processing Science	1,342,000
LIGA Processing	1,058,000
Microstructural and Continuum Evolution Modeling of Sintering	275,000
Biocompatible Self-Assembly of Nano-Materials for Bio-MEMS and Insect Reconnaissance	350,000
Understanding Metal Vaporization from Transient High Fluence Laser Irradiation	85,000
Science Based Processing of Field-Structured Composites	100,000
Design, Synthesis, and Characterization of Soft Matter Nanolayer Superlattices	300,000
Photo-Control of Nano-Interactions in Microsystems	275,000
Electrochemically Deposited Alloys with Tailored Nanostructures for LIGA Micromachines	340,000
Next-Generation Output-Based Process Control: an Integration of Modeling, Sensors, and Intelligent Data Analysis	257,000
Solution-Based Nanoengineering of Materials	320,000
All-Ceramic Thin-Film Battery	310,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$5,732,000
Materials Performance	950,000
High Pressure and Shock Physics	250,000
Aging of Organic Materials	485,000
Corrosion Science and Metal Degradation	135,000
Surface and Interface Reliability	529,000
Nanomechanics	250,000
Micro-Mechanical Behavior and Tribology	200,000
Magnetic-Field Effects on Vacuum-Arc Plasmas	225,000
First-Principles Determination of Dislocation Properties	170,000
Dynamics of Metal/Ceramic Interfaces	160,000
In-Situ Characterization of Soft Solution Processes for Nanoscale Growth	100,000
Determination of Critical Length Scales for Corrosion Processes Using Microelectroanalytical Techniques	160,000
Exploration of New Multivariate Spectral Calibration Algorithms	152,000
Nanostructured Materials for Directed Transport of Excitation Energy	300,000
The Effects of Varying Humidity on Copper Sulfide Film Formation	200,000
Mechanisms of Dislocation-Grain Boundary Interaction	264,000
Physical Basis for Interfacial Traction—Separation Models	297,000
Making the Connection Between Microstructure and Mechanics	257,000
Diagnostics for Joining Solidification/microstructural Simulations	327,000
Effects of Microstructural Variables on the Shock Wave Response of PZT 95/5	321,000

[1]This excludes $51.7 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

NATIONAL NUCLEAR SECURITY ADMINISTRATION (continued)

	FY 2002
OFFICE OF DEFENSE PROGRAMS (continued)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (continued)	
SANDIA NATIONAL LABORATORIES (continued)	
MATERIALS STRUCTURE AND COMPOSITION	$470,000
The Basics of Aqueous Nanofluidics: "Interphase" Structure and Surface Forces	300,000
Modeling Local Chemistry in the Presence of Collective Phenomena	170,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$995,000
Assuring Ultra-Clean Environments in Micro-System Packages: Irreversible and Reversible Getters	365,000
Mechanics and Tribology of MEMS Materials	270,000
LIGA Microsystems Aging: Evaluation and Mitigation	360,000
INSTRUMENTATION AND FACILITIES	$1,235,000
Advanced Analytical Technology Project	735,000
Information Extraction	500,000
LOS ALAMOS NATIONAL LABORATORY	$15,223,000
Enhanced Surveillance Campaign	15,223,000
LAWRENCE LIVERMORE NATIONAL LABORATORY	$5,583,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,750,000
Engineered Nanostructure Laminates	2,750,000
INSTRUMENTATION AND FACILITIES	$2,833,000
AFM Investigations of Biomineralization	113,000
Polyimide Coating Technology for ICF Targets	1,400,000
Beryllium Ablator Coatings for NIF Targets	400,000
Using Dip-Pen Nanolithography to Order Proteins and Colloids at Surfaces	420,000
Plasma Polymer Coating Technology for ICF Targets	500,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION

The mission of the National Nuclear Security Administration is:

- To enhance United States national security through the military application of nuclear energy.
- To maintain and enhance the safety, reliability and performance of the U.S. nuclear weapons stockpile, including the ability to design, produce and test, in order to meet national security requirements.
- To provide the U.S. Navy with safe, militarily effective nuclear propulsion plants and to ensure the safe and reliable operation of those plants.
- To provide international nuclear safety and nonproliferation.
- To reduce global danger from weapons of mass destruction.
- To support U.S. leadership in science and technology.

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 $130.9 million in FY2002. Approximately $51.7 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 Deputy Administrator for Defense Programs within the National Nuclear Security Administration is responsible for carrying out national security objectives established by the President for nuclear weapons and assisting in reducing the global nuclear danger by planning for, maintaining and enhancing the safety, reliability and performance of the U.S. stockpile of nuclear weapons and associated materials, capabilities and technologies in a safe, environmentally sound, and cost-effective manner.

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

313. **MATERIALS SYNTHESIS**
$1,042,000
DOE Contact: Larry Newkirk (202) 586-7831
SNL Contact: B.G. Potter (505) 844-9919 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

314. **METAL PROCESSING SCIENCE**
$1,342,000
DOE Contact: Larry Newkirk (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 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

315. **LIGA PROCESSING**
$1,058,000
DOE Contact: Larry Newkirk (202) 586-7831
SNL Contact: Jill M. Hruby (925) 294-2596 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

316. **MICROSTRUCTURAL AND CONTINUUM EVOLUTION MODELING OF SINTERING**
$275,000
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, are sintered, which is one of the most critical processing steps during ceramic manufacturing. Microstructural evolution, 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. This project is developing 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. This novel modeling method 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

317. **BIOCOMPATIBLE SELF-ASSEMBLY OF NANO-MATERIALS FOR BIO-MEMS AND INSECT RECONNAISSANCE**
$350,000
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 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. 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

318. **UNDERSTANDING METAL VAPORIZATION FROM TRANSIENT HIGH FLUENCE LASER IRRADIATION**
$85,000
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

319. **SCIENCE BASED PROCESSING OF FIELD-STRUCTURED COMPOSITES**
$100,000
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

320. **DESIGN, SYNTHESIS, AND CHARACTERIZATION OF SOFT MATTER NANOLAYER SUPERLATTICES**
$300,000
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 s-polarized 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

321. **PHOTO-CONTROL OF NANO-INTERACTIONS IN MICROSYSTEMS**
$275,000
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. This work 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. Activities 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.

Keywords: Photosensitive, Photonic, Rheology, Polymeric

322. **ELECTROCHEMICALLY DEPOSITED ALLOYS WITH TAILORED NANOSTRUCTURES FOR LIGA MICROMACHINES**
$340,000
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

323. **NEXT-GENERATION OUTPUT-BASED PROCESS CONTROL: AN INTEGRATION OF MODELING, SENSORS, AND INTELLIGENT DATA ANALYSIS**
$257,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Richard A. Neiser (505) 845-0457

The goal of process-based quality is to accept WR (weapon reserve) product without inspection. For simple processes, traditional feedback control of process input variables might achieve this goal. However, input-based (upstream) control systems are a major source of DP production problems for complex processes. With recent advances in sensor technology, process modeling, intelligent data analysis, and computing power, a broadly applicable next-generation control technology that monitors and controls process output rather than input may now be possible. For real-time, output based (downstream) process control, it is necessary to rapidly interpret and correctly respond to large amounts of temporally and spatially varying data, which requires an innovative new approach to data analysis. Highly complex relationships between process inputs and outputs must also be correctly modeled, and cost-effective robust sensors must be developed. In addition, relationships between sensor observations and product microstructure, properties and performance must be understood and integrated into the control system. For some complex processes, e.g., thermal spray, a first-generation downstream process controller based on in-flight monitoring and control of the spray plume may be achievable because some of the requisite technology already exists. To extract needed information from large, rapidly varying, complex data in real-time, we will create a statistical methodology that combines response surface modeling with multivariate statistical process control and a modified simplex search algorithm that incorporates the concept of dynamic annealing.

Keywords: Process Control, Sensors, Process Modeling, Intelligent Data Analysis

324. **SOLUTION-BASED NANOENGINEERING OF MATERIALS**
$320,000
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.

Keywords: Template, Nanostructures, ZnO, Supersaturation

325. **ALL-CERAMIC THIN-FILM BATTERY**
$310,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Timothy J. Boyle (505) 272-7625

The production of a thin-film, all-ceramic battery for power sources that generate the necessary power and energy to operate microsystems without substantially increasing the size of the device are required to achieve autonomy. However, thin-film batteries are currently inadequate to operate the microsystems effectively. We are developing a rechargeable thin-film All-Ceramic Lithium-Ion Battery (ACB) using solution route deposition methods. The ACB will have higher power output, longer run times, and a greatly simplified production scheme in comparison to existing technology. Several ACB prototypes (normal and inverted) have been generated using the above chemistries; however, shorting has complicated the electronic testing. Once sufficiently developed, these ACB will have the versatility to power any number of small systems, such as microsystems and miniature autonomous robotics.

Keywords: Batteries, Microsystems, Thin Films, Lithium Ion Battery

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

326. **MATERIALS PERFORMANCE**
$950,000
DOE Contact: Larry Newkirk (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

327. **HIGH PRESSURE AND SHOCK PHYSICS**
$250,000
DOE Contact: Larry Newkirk (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

328. **AGING OF ORGANIC MATERIALS**
$485,000
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

329. **CORROSION SCIENCE AND METAL DEGRADATION**
$135,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: 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

330. **SURFACE AND INTERFACE RELIABILITY**
$529,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Kevin F. McCarty (925) 294-2067

The engineered microstructures of metals enable the performance of many non-nuclear components in nuclear weapons. Time-dependent changes of microstructure can lead to failure of stockpile components. A new and large issue that needs to be addressed is the aging (dormancy) of microsystem parts produced by the LIGA process, which uses electrodeposition for part fabrication. Because of the central role of microstructure in stockpile components and anticipated replacement components based on microsystems, this research task is focused on some of the fundamental aspects of metal microstructure. We emphasize the relationship between microstructure and mechanical properties such as yield strength. To develop predictive capability for performance and lifetime, we perform both simulation and experiment. This task has three major thrusts: 1) grain-boundary structure and dynamics, 2) microstructure of electrodeposited metals, and 3) computational-technique development.

Keywords: Time-Dependent, Microstructure, Electrodeposition, Lifetime, Grain-Boundary

331. **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

332. **MICRO-MECHANICAL BEHAVIOR AND TRIBOLOGY**
$200,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Jonathan S. Custer (505) 845-8594

The goal of this project is to improve the fundamental understanding of the microstructural mechanisms and topographical features that control mechanical and tribological behavior of materials. Tools and techniques will be developed to measure materials performance at length scales that are consistent with microstructural dimensions.

Keywords: Mechanical, Topographical, Tribological, Microstructural, Microsystem

333. **MAGNETIC-FIELD EFFECTS ON VACUUM-ARC PLASMAS**
$225,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Paul A. Miller (505) 844-8879

The 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. 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. 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. 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.

Keywords: Vacuum-Arc Plasmas, Magnetic Fields, Plasma Plume, Langmuir Probe

334. **FIRST-PRINCIPLES DETERMINATION OF DISLOCATION PROPERTIES**
$170,000
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 presence of defects is central to developing predictive models of material evolution. 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 dislocation 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. We will 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. Additional modeling using an *ab-initio* extension of Peierls-Nabarro is also being 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

335. **DYNAMICS OF METAL/CERAMIC INTERFACES**
$160,000
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

336. **IN-SITU CHARACTERIZATION OF SOFT SOLUTION PROCESSES FOR NANOSCALE GROWTH**
$100,000
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 following the development of supersaturation, surface processes, and formation of a precipitating system *in-situ*. This proposal will study the superposition of different measurement techniques to characterize dynamic colloidal systems in novel ways. These studies will probe the chemical interactions during reactions, and the organizational characteristics developed in the resulting colloids.

Keywords: Nanomaterials, Soft Solution Processes, Colloids

337. **DETERMINATION OF CRITICAL LENGTH SCALES FOR CORROSION PROCESSES USING MICROELECTROANALYTICAL TECHNIQUES**
$160,000
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 work focuses on two areas of corrosion science, where a fundamental understanding of processes occurring at critical dimensions is 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. 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. 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

338. **EXPLORATION OF NEW MULTIVARIATE SPECTRAL CALIBRATION ALGORITHMS**
$152,000
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. 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

339. **NANOSTRUCTURED MATERIALS FOR DIRECTED TRANSPORT OF EXCITATION ENERGY**
$300,000
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

340. **THE EFFECTS OF VARYING HUMIDITY ON COPPER SULFIDE FILM FORMATION**
$200,000
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

341. **MECHANISMS OF DISLOCATION-GRAIN BOUNDARY INTERACTION**
$264,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Robert Q. Hwang (925) 294-1570

Incorporating the localized atomistic and microscopic effects of internal interfaces on materials properties and long-term behavior is a significant challenge for large-scale materials simulations. Critical to improving such models is developing an improved understanding of the dislocation-grain boundary interactions that ultimately control the interfacial response to strain. Such interactions impact many materials phenomena and properties including slip transmission, boundary migration, recrystallization, and yield strength and are a critical element in linking atomic structure to continuum behavior. In this project we seek to develop an experimentally based understanding of these dislocation-grain boundary interactions.

Keywords: Dislocation, Grain Boundary

342. **PHYSICAL BASIS FOR INTERFACIAL TRACTION - SEPARATION MODELS**
$297,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: E.David Reedy (505) 844-3297

Many components contain interfaces between dissimilar materials where cracks can initiate and fail components. In recent years, researchers in the fracture community have adopted a cohesive zone model for simulating crack propagation (based upon traction-separation relations). Sandia is implementing this model in its ASCI codes. However, one important obstacle to using a cohesive zone modeling approach is that traction-separation relations are chosen in an ad hoc manner. The goal of the present work is to determine a physical basis for mesoscale level Traction-Separation (T-U) relations. We propose experiments that will elucidate the dependence of such relations on adhesive and bulk properties. Work will focus on epoxy/solid interfaces, although the approach is applicable to a broad range of materials. The crucial roles of crack tip plastic zone size and interfacial adhesion are being defined by varying epoxy layer thickness and using coupling agents or special self-assembled monolayers (SAMs) in preparing samples. The nature of the yield zone will be probed in collaborative experiments run at the Advanced Photon Source, and high-resolution optical methods will be used to measure crack opening displacements of the SDCB specimens. This work will provide an understanding of the major mesoscale phenomena governing polymer/solid interfacial fracture and identify the essential features that must be incorporated in a T-U based cohesive zone failure model. We believe that models using physically based T-U relations will provide an essential tool for using models to tailor interface properties to meet design needs.

Keywords: Traction-Separation, Interfacial Fracture

343. **MAKING THE CONNECTION BETWEEN MICROSTRUCTURE AND MECHANICS**
$257,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Elizabeth A. Holm (505) 844-7669

The purpose of microstructural control is to optimize materials properties. To that end, we have developed sophisticated and successful computational models of both microstructural evolution and mechanical response. However there is currently no way to couple these models to quantitatively predict the properties of a given microstructure. The problem arises because continuous response models, such as finite element, finite volume, or materials point methods, do not incorporate a real length scale. In this project, we are taking a tiered risk approach to incorporate microstructure and its resultant length scales in mechanical response simulations. The successful coupled model will predict both properties as a function of microstructure and microstructural development as a function of processing conditions.

Keywords: Microstructure, Mechanical Properties, Computational Materials Science

344. **DIAGNOSTICS FOR JOINING SOLIDIFICATION/MICROSTRUCTURAL SIMULATIONS**
$327,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: Charles V. Robino (505) 844-6557

Solidification is an important aspect of welding, brazing, soldering, LENS fabrication, and casting. For these processes solidification affects, and in many instances controls, the final microstructure and properties of the product. The current trend toward utilizing large-scale process simulations and materials response models for simulation-based engineering is driving the development of new modeling techniques. However, the effective utilization of these models and simulations is currently limited by a lack of fundamental understanding of the sub-processes and interactions involved. This project is identifying key physical phenomena in, and expanding and refining our mechanistic descriptions of, solidification in the Fe-Cr-Ni system. The experimental study is coupled to modeling efforts focused on solidification processes in the same alloy system, and provides necessary mechanistic descriptions and input data for these models. We have developed and will continue to refine new and expanded experimental techniques, particularly those needed for *in-situ* measurement of the kinetics features of the solidification process. This approach has identified several unexpected features of the solidification process, including the observation that the solidification front is more dynamic than previously thought and the observation of a previously unreported orientation relationship between ferrite and austenite.

Keywords: Solidification, Ferrite, Austenite, Joining

345. **EFFECTS OF MICROSTRUCTURAL VARIABLES ON THE SHOCK WAVE RESPONSE OF PZT 95/5**
$321,000
DOE Contact: Gerald Green (202) 586-8377
SNL Contact: George A. Samara (505) 844-6653

Sandia has responsibility for the design and production of neutron generators. Most generators use explosively driven power supplies in which shock wave depoling of the ferroelectric ceramic PZT 95/5 provides the required high voltage for the neutron tube. Generator production will change within a few years to PZT 95/5 material prepared using a new "chem prep" process that is still under development. This process will introduce a porous microstructure that is significantly different than that found within most material presently in the stockpile. Early studies showed that the porous microstructure can have a profound effect on performance: the rate for failures due to high-voltage breakdown at low temperatures is acceptably low only in materials made within a narrow density range through the addition of organic pore formers. More fundamentally, the dielectric and ferroelectric properties of the material and the physics of the FE (ferroelectric)-to-AFE (antiferroelectric) phase transformation that governs the depoling process depend on microstructural properties in ways that are not well understood. This project represents the first systematic study of the basic physics of microstructural effects on PZT 95/5 electromechanical behavior under shock loading. Dielectric properties are characterized for material samples having different densities, and the electromechanical responses of similar samples are investigated under carefully controlled shock loading conditions. Results to date demonstrate significant porosity effects on both the dynamic material response and shock-induced depoling, provide insight into a recently confirmed failure mechanism, and underscore the continuing need for systematically examining microstructural variables.

Keywords: Shock Wave Depoling, Ferroelectric, PZT 95/5, Phase Transition

MATERIALS STRUCTURE AND COMPOSITION

346. **THE BASICS OF AQUEOUS NANOFLUIDICS: "INTERPHASE" STRUCTURE AND SURFACE FORCES**
$300,000
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

347. **MODELING LOCAL CHEMISTRY IN THE PRESENCE OF COLLECTIVE PHENOMENA**
$170,000
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

348. **ASSURING ULTRA-CLEAN ENVIRONMENTS IN MICRO-SYSTEM PACKAGES: IRREVERSIBLE AND REVERSIBLE GETTERS**
$365,000
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 and particulates. 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. 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 reactive 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. 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.

Keywords: Getter, Microdevices, Packaging, Absorption

349. **MECHANICS AND TRIBOLOGY OF MEMS MATERIALS**
$270,000
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. 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

350. **LIGA MICROSYSTEMS AGING: EVALUATION AND MITIGATION**
$360,000
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 and contact with other metallic structures. We propose to characterize LIGA materials, 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

INSTRUMENTATION AND FACILITIES

351. **ADVANCED ANALYTICAL TECHNOLOGY PROJECT**
$735,000
DOE Contact: Syed Zaidi (301) 903-3446
SNL Contact: Raymond P. Goehner
(505) 844-9200

Our goal is to develop 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) microstructural 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; 2) application and development of spectrum imaging techniques applied to electron microscopes equipped with X-ray and electron energy loss spectrometers and three-dimensional spectrum imaging of near-surface regions and larger volumes; 3) improve 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

352. **INFORMATION EXTRACTION**
$500,000
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 AFM/FTIR, a combination of atomic force microscopy (AFM) technology with a Fourier transform infrared (FTIR) source for high resolution analysis. Also, techniques using photoacoustic infrared spectroscopy (PAS) and Raman imaging will be developed for analysis of polymeric materials, and silicon microsystems, respectively.

Keywords: Algorithms, Multivariate Analysis, Spectroscopy, AFM/FTIR

LOS ALAMOS NATIONAL LABORATORY

353. **ENHANCED SURVEILLANCE CAMPAIGN**
$15,223,000
DOE Contacts: E. Cochran (301) 903-7330 and S. Zaidi (301) 903-3446
LANL Contacts: K. B. Alexander (505) 665-4750 and R. Krabill (505) 667-4286

The Stockpile Surveillance Program provides protection to the U.S. nuclear weapons stockpile by an intensive program that assures it is free of defects that may affect performance, safety, or reliability. It consists of two elements, the Stockpile Evaluation Program and the Enhanced Surveillance Campaign. The Stockpile Evaluation Program provides the examinations and assessments of WR stockpile weapons and components. The Enhanced Surveillance Program provides means to strengthen the Stockpile Evaluation Program to meet the challenges of an aging stockpile in an era of no nuclear testing as well as providing lifetime assessments and predictions for lifetime extension program (LEP) planning.

The Enhanced Surveillance Campaign will protect the health of the stockpile by providing advance warning of manufacturing and aging defects to allow refurbishment before performance is impaired. The Campaign will provide diagnostics for screening of weapons systems to identify units that must be refurbished as well as for early detection of defects. It will also predict material and component aging rates as a basis for annual certification, refurbishment scope and timing, and nuclear weapon complex planning. Results of the work will include improvements to the basic Surveillance Program. Since nuclear weapons will be retained in the stockpile for lifetimes beyond our experience, the Department of Energy (DOE) needs a firm basis on which to determine when stockpile systems must be refurbished or reconditioned. If new refurbishment capability is needed, the DOE needs to know:

- When these capabilities must be operational and what the required capacity should be
- If the capacity for existing facilities is adequate and when potential refurbishment for the various stockpile systems must be scheduled
- A basis from which to characterize the functional reliability of aged components, as part of the annual assessment process

The work in the ES Campaign began in late FY97. The principal milestones and deliverables for this campaign are below:

- Provide a stockpile aging assessment annually for use in performing the annual assessment of the stockpile annually)
- Provide component lifetime assessments for weapon refurbishments to enable component replacement decisions and age-aware component design and material selections
- Provide data or requirements to enable facility planning, design, and construction
- Develop validated models for the aging of materials, components, and systems for use in weapon certification
- Deliver advanced diagnostic tools to enable more predictive, higher fidelity, and non-destructive surveillance test capability

Our work is divided into five major technical elements (MTE): pits, CSAs/Cases, high explosives (HE), systems, and non-nuclear materials (NNM). The pit, CSA/Cases, and high explosives MTEs are each divided into two projects; lifetime assessments and diagnostics. The Systems MTE is responsible for assessments/ methodologies to support decision making under uncertainty. The Non-nuclear materials MTE is divided into two projects; material lifetimes and advanced diagnostic tools.

Complete details for the Enhanced Surveillance Campaign can be found in the ESC Program Plan and the ESC Implementation Plan, which are updated on a yearly basis.

Keywords: Nuclear Weapons, Pits, Plutonium, CSA, Canned Subassembly, High Explosives, Non-Nuclear Materials, Systems, Reliability, Energetic Materials, Stockpile, Enhanced Surveillance, Campaign 8, Accelerated Aging, Lifetime prediction, Aging

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

354. **ENGINEERED NANOSTRUCTURE LAMINATES**
$2,750,000
DOE Contact: 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 and energetic materials development.

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.

Keywords: Precision Thin Films, Multilayer Technology, Passive Elecrtonic Devices, Energetic Materials, IR, Visible, UV, EUV, SXR and XR Optics, Optic Systems

INSTRUMENTATION AND FACILITIES

355. **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

356. **POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS**
$1,400,000
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. The focus of the past year has been improvement of the capsule surface finish.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

357. **BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS**
$400,000
DOE Contact: Bharat Agrawal (301) 903-2057
LLNL Contacts: R. McEachern (925) 423-4734, R. Cook (925) 422-3117 and R. Wallace (925) 423-7864

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

358. **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

359. **PLASMA POLYMER COATING TECHNOLOGY FOR ICF TARGETS**
$500,000
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(a-methylstyrene) 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. The focus of the past year has been improvement of the mandrel surface finish.

Keywords: Polymers, Laser Fusion Targets, Plasma Polymer, Ablator

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

	FY 2002
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT - GRAND TOTAL	$30,540,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$30,540,000
Waste Packages	30,540,000

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

360. **WASTE PACKAGES**
$30,540,000
DOE Contact: Paige Russell, (702) 794-1315 and Kirk Lachman, (702) 794-5096
M&O Contacts: Larry Lucas, (702) 295-4414 and Robert Andrews, (702) 295-5549

The development of the nation's high-level waste repository has been delegated to DOE's Yucca Mountain Site Characterization Project Office. Bechtel SAIC Company, the contractor for the Civilian Radioactive Waste Management System, is responsible for designing the waste package and related portions of the engineered barrier system. The advanced conceptual design was completed in 1996 and Viability Assessment design was completed in 1998. The current design was selected in 1999. Progress on the waste package and the supporting materials studies has been documented in various reports.

The waste package design effort includes the development of waste packages to accommodate uncanistered commercial spent nuclear fuel (SNF),canistered SNF, canistered defense high-level waste, Navy fuel, and other DOE-owned spent nuclear fuel. The analytical process that is underway to support these designs included thermal, structural, and neutronic analyses. Also included are materials selection and engineering development. The current design consists of a corrosion-resistant outer barrier of Alloy 22 and a stainless steel inner shell, which provides structural support. Titanium is still used as the drip shield material.

The waste package materials effort includes the testing and modeling of materials being considered for inclusion in the waste package and the engineered barrier system. These materials include Alloy 22 (UNS# N06022), titanium grade 7, titanium grade 24, and 316 stainless steel. The testing includes general aqueous and humid air testing, localized degradation such as pitting and crevice corrosion, micro-biologically-influenced corrosion, galvanic corrosion, and stress corrosion cracking. The corrosion test facility started the long-term test program in FY 1997. Evaluation of five-year specimens will be initiated in FY 2003. Waste form materials are also being evaluated for alteration and leaching under repository-relevant conditions. In 2002 the short-term test program was continued to support waste package material degradation model development effort. The short-term test program focuses on stress corrosion cracking, crevice corrosion, and passive film stability among the candidate materials.

Keywords: Yucca Mountain Repository, Waste Package, Engineered Barrier System

OFFICE OF FOSSIL ENERGY

	FY 2002
OFFICE OF FOSSIL ENERGY - GRAND TOTAL	$10,343,999
OFFICE OF ADVANCED RESEARCH	$10,343,999
FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM	$6,745,999
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$2,450,000
Mo-Si Alloy Development	300,000
Influence of Processing on Microstructure and Properties of Intermetallics	170,000
Chemically Vapor Deposited YSZ for Thermal and Environmental Barrier Coatings	225,000
Corrosion-Resistant Composite Structures	275,000
Extended-Lifetime Metallic Coatings for High-Temperature Environmental Protection	210,000
Evaluation of Advanced Pressure Boundary Alloys for Heat Recovery Systems	190,000
Intermetallic Reinforced Cr Alloys	110,000
Development of Novel Activated Carbon Composites	200,000
Corrosion Protection of Ultrahigh Temperature Intermetallic Alloys	200,000
CRADAs for Development and Testing of Carbon Materials	150,000
CRADA on Advanced Austenitic Alloys	50,000
CRADA on Thermie Alloy Processing	70,000
Development of VLS Scaling Parameters for Production of Silicon Carbide Fibrils	125,000
Metallic Coatings for Power-Generation Applications	85,000
Modeling of CVD for Solid State Electrolytes	90,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,160,000
Development of NDE Methods for Structural Ceramics	175,000
Corrosion and Mechanical Properties of Alloys in FBC and Mixed-Gas Environments	175,000
Investigation of the Weldability of Intermetallics	70,000
In-Plant Corrosion Probe Tests of Advanced Austenitic Alloys	80,000
Investigation of Weld Overlays and Coatings	100,000
Oxide Dispersion Strengthened (ODS) Alloys	230,000
Concepts for Smart Protective High-Temperature Coatings	70,000
Reduction of Defect Content In ODS Alloys	100,000
Support Services for Ceramic Hot-Gas Filters and Heat Exchangers	100,000
Intrinsic and Extrinsic Fracture Behavior of Intermetallic Compounds	60,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$2,480,000
Metallic Filters for Hot-Gas Cleaning	90,000
Refractory Materials Issues in Gasifiers	100,000
Development of Ceramic Membranes for Hydrogen Separation	350,000
Production of Pure Hydrogen from Hydrocarbons	100,000
Materials and Components in Fossil Energy Applications Newsletter	60,000
High-Temperature Materials Testing in Coal Combustion Environments	200,000
Improved Membrane Materials and Economical Fabrication	225,000
Management of Advanced Research Materials Program	400,000
Membrane Seal Development, Characterization, and Testing	450,000
Personal Services Contract	20,000
Development of ODS Alloy for Heat Exchanger Tubing	160,000
Molecular Sieves for Hydrogen Separation	150,000
Microscopic and Microstructural Issues for Optimal Material Design	100,000
Fatigue and Fracture Behavior of Cr-X Alloys	75,000

OFFICE OF FOSSIL ENERGY (continued)

	FY 2002
FOSSIL ENERGY ADVANCED RESEARCH MATERIALS PROGRAM (continued)	
ULTRA-SUPERCRITICAL STEAM POWER PLANT RESEARCH	$550,000
Ultra-Supercritical Steam Turbine Materials	200,000
Materials for Ultra-Supercritical Steam Power Plants	0
Ultra-Supercritical Steam Cycle Turbine Materials	350,000
VISION 21 SUPPORT ACTIVITIES	$105,999
Improved ODS Alloy for Heat Exchanger Tubing	105,999
ADVANCED METALLURGICAL PROCESSES PROGRAM	$3,598,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$960,000
Advanced Foil Lamination Technology	560,000
Advanced Casting Technologies	400,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,638,000
Advanced Refractories for Gasifiers	600,000
Oxidation and Sulfidation Resistant Materials	600,000
Wear and Abrasion of Materials for Fossil Energy Systems	600,000
Mechanisms of Corrosion Under Ash Deposits	550,000
Non-Isothermal Corrosion and Oxidation	288,000

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

FOSSIL ENERGY 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

361. **Mo-Si ALLOY DEVELOPMENT**
$300,000
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 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

362. **INFLUENCE OF PROCESSING ON MICROSTRUCTURE AND PROPERTIES OF INTERMETALLICS**
$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

The objective of this program is to develop techniques for processing advanced alloys for fossil energy applications to improve elevated temperature mechanical properties and resistance to environmental degradation. Extensive work has been performed in cooperation with the efforts at ORNL on development: of aluminide alloys for structural applications. Significant progress has been made on improving the ambient temperature ductility and creep properties of these alloys. It has been determined that much of the benefit of environmental resistance from these alloys could be obtained from coatings. Results on the relationship of processing to microstructure, properties and performance of iron aluminides will be extended to coatings for protection of structural alloys from environmental degradation. Advanced in situ diagnostics will be employed to determine the relationship of particle characteristics size, temperature and velocity during thermal spray deposition to the observed residual stress and microstructure. The environmental resistance of these well characterized coatings to high temperature atmospheres of interest to fossil energy applications will be determined in collaboration with ORNL. Coating synthesis and performance characteristics of other advanced alloys, e.g., Mo-Si- and chromia-forming alloys will also be examined.

Keywords: Aluminides, Processing, Microstructure

363. **CHEMICALLY VAPOR DEPOSITED YSZ FOR THERMAL AND ENVIRONMENTAL BARRIER COATINGS**
$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

364. **CORROSION-RESISTANT COMPOSITE STRUCTURES**
$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: Composites, Ceramics, Fiber-Reinforced, Corrosion

365. **EXTENDED-LIFETIME METALLIC COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL PROTECTION**
$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

366. **EVALUATION OF ADVANCED PRESSURE BOUNDARY ALLOYS FOR HEAT RECOVERY SYSTEMS** $190,000
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: 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 750˚C and higher.

Keywords: Materials, Mechanical Properties, Austenitics, Hot-Gas

367. **INTERMETALLIC REINFORCED Cr ALLOYS** $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. The effort will initially be devoted to in-situ composite alloys based on a Cr solid solution matrix reinforced with intermetallic Cr_2X (X = Nb, Ta, Y) Laves phases. A major goal of this program will be to transition the advances made in identifying, understanding and developing new families of high-performance multi-phase alloys to applied spin-off efforts devoted to further alloy/coating development and optimization for specific energy conversion and combustion system applications and components.

Keywords: Alloys, Chromium-Niobium, Corrosion, Intermetallic Compounds

368. **DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES**
$200,000
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. D. Burchell (865) 576-8595

There is increasing interest in the separation of CO_2 from a variety of gas streams and for a variety of purposes. The separations include the removal of CO_2 from gas turbine exhaust gas streams for subsequent disposal (e.g., by injection into an oil well for enhanced oil recovery), or the removal of CO_2 from the fuel and oxidant streams of fuel cells. Moreover, natural gas frequently contains large fractions of diluents and contaminants such as CO_2 and H_2S. Carbon Fiber Composite Molecular Sieves (CFCMS) materials will be developed to effect the separation of diluents and contaminants from natural gas. Additionally, H_2O must be removed from natural gas to minimize pipeline corrosion. The purpose of this work is to develop carbon molecular sieves (CMS) starting with porous Carbon Fiber Composites (CFC) manufactured from petroleum pitch derived carbon fibers. The CFCMS will be utilized in Pressure Swing Adsorption (PSA) units or Electrical Swing Adsorption (ESA) units for the efficient recovery of CO_2 from gas mixtures. Novel separation techniques, that exploit the unique combination of properties of CFCMS, will be developed to effect the above mentioned separations.

Keywords: Carbon Fibers, Sieves, Composites

369. **CORROSION PROTECTION OF ULTRAHIGH TEMPERATURE INTERMETALLIC ALLOYS**
$200,000
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 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. The effort will initially be devoted to in-situ composite alloys based on a Cr solid solution matrix reinforced with intermetallic Cr_2X (X = Nb, Ta, Y) Laves phases. A major goal of this program will be to transition the advances made in identifying, understanding and developing new families of high-performance multi-phase alloys to applied spin-off efforts devoted to further alloy/coating development and optimization for specific energy conversion and combustion system applications and components.

Keywords: Coatings, Corrosion

370. **CRADAS FOR DEVELOPMENT AND TESTING OF CARBON MATERIALS**
$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:
T. D. Burchell (865) 576-8595

Hydrogen and methane gas recovery technologies are required to: 1) allow the upgrading of heavy hydrocarbons to transport fuels, thus reducing the amount of carbon rejected during crude oil refining and 2) improve the yield and process economics of natural gas wells. The purpose of this work is to develop carbon fiber composite molecular sieves (CFCMS) from porous carbon fiber composites manufactured from solvent extracted coal tar pitch derived carbon fibers.

Keywords: Carbon Products

371. **CRADA ON ADVANCED AUSTENITIC ALLOYS**
$50,000
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:
R. W. Swindeman (865) 574-5108

The purpose of this task is to engage in cooperative work with an industrial firm on the development of advanced austenitic alloys.

Keywords: Alloys, Austenitics, Technology Transfer

372. **CRADA ON THERMIE ALLOY PROCESSING**
$70,000
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:
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: Alloys, Technology Transfer

373. **DEVELOPMENT OF VLS SCALING PARAMETERS FOR PRODUCTION OF SILICON CARBIDE FIBRILS**
$125,000
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
ReMaxCo Technologies, Inc. Contact:
R. D. Nixdorf (865) 483-5060

The DOE Fossil Energy Program has an interest in silicon carbide fibrils as a material for high-temperature heat exchanger and recuperation components in advanced coal combustion plants. The purpose of this project is to develop a commercial process for the production of silicon carbide fibrils. The slow growth of the fibrils and excessive waste of raw materials have been the major impediments. This work is an effort to bring new technology solutions to the future volume production of silicon carbide fibrils.

Keywords: Ceramics, Composites, Fibrils, Modeling

374. **METALLIC COATINGS FOR POWER-GENERATION APPLICATIONS**
$85,000
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
Tennessee Technological University Contact:
Ying Zhang (931) 372-3186

The purpose of this task 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: Coatings, Corrosion

375. **MODELING OF CVD FOR SOLID STATE ELECTROLYTES**
$90,000
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
University of Louisville Contact: T. L. Starr
(502) 852-1073

There are two critical requirements for successful, ambient pressure CVD of solid oxide electrolyte films: maintain uniformity in thickness and composition over a reasonably large substrate, and avoid gas-phase nucleation that degrades film quality. The proposed research addresses both requirements and is based on the unique characteristics of stagnation point flow.

Stagnation point flow describes the characteristics of a fluid stream impinging upon a planar substrate. With this geometry, modeling of mass and energy transport between the stream and the substrate surface can be reduced to a one-dimensional, boundary layer problem. Further, with proper selection of flow conditions, the effective boundary layer thickness is essentially uniform over an appreciable portion of the substrate. Also, by utilizing a cold-wall design—cool stream impinging on a heated substrate—the "residence time at temperature" for the stream is small, minimizing gas phase reactions.

This project shall investigate the application of stagnation point flow to the deposition of yttrium-stabilized zirconia (YSZ) solid electrolyte films, including an experimental effort at ORNL and a modeling effort at the University of Louisville.

Keywords: Ceramics, Composites, Modeling, Fuel Cells

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

376. **DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS FOR STRUCTURAL CERAMICS**
$175,000
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
Argonne National Laboratory Contact:
W. A. Ellingson (630) 252-5068

The purpose of the work in this project is to develop nondestructive evaluation (NDE) technology as part of the overall effort to develop high temperature materials for advancing utilization of fossil fuel resources. This work focuses on advanced structural and functional materials used to foster clean utilization of coal. These new high-temperature materials, which are an enabling technology, will allow coal to be utilized in a more environmentally acceptable manner. Examples of high-temperature ceramics include high-temperature 0_2 and H_2 separation membranes and thermal barrier coatings for first-stage hot-section blades and vanes in combustion turbines. The NDE technology provides end users with reliable data on which to make cost-effective decisions about whether to replace a component or allow a component to remain in service. In addition, the NDE data may be coupled with models for predicting the remaining life of a particular component.

Keywords: Nondestructive Evaluation, Ceramics, Flaws, Fracture

377. **CORROSION AND MECHANICAL PROPERTIES OF ALLOYS IN FBC AND MIXED-GAS ENVIRONMENTS**
$175,000
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
Argonne National Laboratory Contact: K. Natesan
(630) 252-5103

The purposes of this task are: 1) to evaluate the corrosion performance of materials in simulated combustion environments for application in advanced steam-cycle systems, 2) to evaluate the role of deposits containing sulfur and/or chlorine and ash constituents in the corrosion behavior of metallic alloys, selected coatings, and monolithic/composite ceramics, 3) to evaluate the residual mechanical properties of materials after exposure in corrosive environments and quantify the effects of corrosion on the properties to enable life prediction of components, and 4) to expose candidate alloys, coatings, weldments, and ceramics in small-scale combustion test facilities at the NETL and the University of North Dakota Energy and Environmental Research Center.

Keywords: Corrosion, Gasification, Creep Rupture, Fluidized-Bed Combustion

378. **INVESTIGATION OF THE WELDABILITY OF INTERMETALLICS**
$70,000
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
Colorado School of Mines Contact: G. R. Edwards (303) 273-3773

The purpose of this project is the investigation of the weldability of polycrystalline aluminides. The major thrust of the project is to determine the role of microstructure in the intergranular cracking of aluminides, with special emphasis on weld cracking susceptibility. The weldability of polycrystalline Fe_3Al-X alloys is being evaluated, and the weldability is correlated with composition, phase equilibria, grain size and morphology, domain size, and degree of long-range order.

Keywords: Joining, Welding

379. **IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS**
$80,000
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
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: Austenitics, Alloys, Corrosion

380. **INVESTIGATION OF WELD OVERLAYS AND COATINGS**
$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: A. R. Marder (610) 758-4197

The objective of this activity is the investigation of iron aluminide weld overlays. Specific tasks include: 1) filler wire development 2) weldability 3) oxidation and sulfidation studies 4) erosion studies 5) erosion-corrosion studies, and 6) field exposures.

Keywords: Alloys, Aluminides, Overlay, Welding, Joining

381. **OXIDE DISPERSION STRENGTHENED (ODS) ALLOYS**
$230,000
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 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: Aluminides

382. **CONCEPTS FOR SMART PROTECTIVE HIGH-TEMPERATURE COATINGS**
$70,000
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 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, Corrosion

383. **REDUCTION OF DEFECT CONTENT IN ODS ALLOYS**
$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
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: Aluminides, Defects

384. **SUPPORT SERVICES FOR CERAMIC HOT-GAS FILTERS AND HEAT EXCHANGERS**
$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
University of North Dakota Energy and
Environmental Research Center (UNDEERC)
Contact: J. P. Hurley (701) 777-5159

This task will review and, if appropriate, propose modifications to plans, materials, and tests planned by researchers on the Advanced Research Materials Program in work to test materials for coal-fueled energy systems. The changes shall be suggested in order to make the corrosion experiments more reflective of the actual conditions that will be encountered by the materials in the energy systems. UNDEERC shall accomplish this task by reviewing the major advanced energy system projects being funded by the DOE, and by working with the company's technical monitor and staff to prepare a summary of the expected corrosion problems. Both gasification and combustion systems will be included. Ceramic materials in two subsystems will be the focus of this work: 1) hot gas cleanup systems and 2) high-temperature heat exchangers. UNDEERC shall review and suggest improvements to materials testing procedures that are used to determine material behavior when used in hot-gas cleanup or heat exchanger applications. A limited amount of computer modeling and laboratory experimentation shall be a part of this effort.

Keywords: Composites, Ceramics, Fibers

385. **INTRINSIC AND EXTRINSIC FRACTURE BEHAVIOR OF INTERMETALLIC COMPOUNDS**
$60,000
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
West Virginia University Contact: B. R. Cooper
(304) 293-3423

The purpose of this activity is the evaluation of the intrinsic and extrinsic fracture behavior of iron aluminides and the study of atomistic simulations of defect concentrations, dislocation mobility, and solute effects in Fe_3Al. The work also involves an experimental study of environmentally-assisted crack growth of Fe_3Al at room and at elevated temperatures. The combined modeling and experimental activities are expected to elucidate the mechanisms controlling deformation and fracture in Fe_3Al in various environments.

Keywords: Alloys, Aluminides, Fracture

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

386. **METALLIC FILTERS FOR HOT-GAS CLEANING**
$90,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Ames Laboratory Contact: Iver Anderson
(515) 294-4446

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

387. **REFRACTORY MATERIALS ISSUES IN GASIFIERS**
$100,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Albany Research Center Contact:
Richard P. Walters (541) 967-5873

The purpose of this research is to characterize and understand slag component interactions with the refractories used in coal gasifiers. It is anticipated that once these interactions are understood, it will be possible to find a means of controlling, i.e., limiting, the slag-refractory interactions and extending the refractory lifetime.

Keywords: Refractories

388. **DEVELOPMENT OF CERAMIC MEMBRANES FOR HYDROGEN SEPARATION**
$350,000
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:
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, Filters, Separation

389. **PRODUCTION OF PURE HYDROGEN FROM HYDROCARBONS**
$100,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
Los Alamos National Laboratory Contact:
Steven A. Birdsell (505) 667-5868

The palladium membrane reactor was developed for processing tritiated water and tritiated hydrocarbons found in fusion energy, weapons and environmental applications. In addition to these applications, the PMR has the potential to revolutionize fossil fuel processing. However, in order to use the PMR in fuel applications, further performance data and development are needed. A state-of-the art PMR employing a thin palladium (Pd) film composite membrane will be used to evaluate performance and determine the best operating conditions for production of pure hydrogen from coal gas. Simulated coal-gas processing has been done at higher pressures (> 200 psig). Real coal gas contains impurities such as sulfur that are potentially poisonous to PMRs. This effect will need to be determined. Also, in order to make the technology practical for industrial use, a higher flux Pd membrane is needed. Such a membrane has been developed at Los Alamos. An advanced PMR will be constructed with the high-flux membrane and tested with simulated coal gas. Successful demonstration of the advanced PMR could lead to a radical decrease in the cost of fossil fuel processing. The purpose of this project is to develop palladium membrane reactor (PMR) technology for production of hydrogen from coal gas.

Keywords: Membranes

390. ***MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS* NEWSLETTER**
$60,000[1]
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 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: Materials, Components

391. **HIGH-TEMPERATURE MATERIALS TESTING IN COAL COMBUSTION ENVIRONMENTS**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
National Energy Technology Laboratory Contact:
Anthony V. Cugini (412) 892-6023

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 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

[1]Matching funding provided by EPRI.

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: Testing

392. **IMPROVED MEMBRANE MATERIALS AND ECONOMICAL FABRICATION**
$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. R. Armstrong (865) 574-7996

The purpose of this task is to develop infrared plasma processing as a method to rapidly sinter membrane materials such as yttria stabilized zirconia (YSZ, for fuel cells) and barium cerate (for hydrogen separation). This process will fully evaluate and determine the feasibility of this process for sintering YSZ and barium cerate films deposited by screen printing on green and pre sintered support structures. The goal of this process is to reduced cycle times and costs for membrane fabrication. In addition, this task will start pursuing development of novel approach for the fabrication of asymmetric membranes.

Keywords: Membranes

393. **MANAGEMENT OF THE ADVANCED RESEARCH MATERIALS PROGRAM**
$400,000
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:
R. R. Judkins (865) 574-4572

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 (ORNL) 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.

Keywords: Management, Materials Program

394. **MEMBRANE SEAL DEVELOPMENT, CHARACTERIZATION, AND TESTING**
$450,000
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:
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 Testing, Seals

395. **PERSONAL SERVICES CONTRACT**
$20,000
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. T. Carlson (865) 574-5135

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: Conference, Exhibits

396. **DEVELOPMENT OF ODS ALLOY FOR HEAT EXCHANGER TUBING**
$160,000
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
Special Metals Corporation Contact: Mark Harper (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: Alloys, Tubing

397. **MOLECULAR SIEVES FOR HYDROGEN SEPARATION**
$150,000
DOE Contacts: F. M. Glaser (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
Sandia National Laboratories Contact: Anthony Martino (505) 844-3332

The purpose of this program is to develop and test three novel inorganic-organic materials for hydrogen separation and purification. The program will combine experimental and theoretical efforts to develop and test the following three materials as the working thin film in asymmetric Interfacial composite membranes (on alumina supports): *In situ* generated bridged polysilsesquioxanes, organic templated silicates and catalytic membranes. 1) Bridged polysilsesquioxanes belong to a class of hybrid organic-inorganic materials with thermal stability to 500°C and resistance to acids, strong bases and organic solvents. The organic bridging group can be varied to give an enormous range of materials with differing physical and chemical properties, including hydrogen permeation
2) Organic templated silicates are designed to exhibit greater thermal and chemical stability while still forming the molecular sieving layer in asymmetric membranes. These materials are prepared from silane precursors whose organic group chemically reacts during the membrane formation to generate the membrane. 3) We will team these synthetic strategies with catalyst syntheses such as micelle-mediated preparation of metal nanoclusters to generate a revolutionary catalyst separation system combining highly dispersed metal nanoclusters in hybrid membranes with precisely modulated permselectivity. These catalytic membranes will provide a technology to perform reactions such as hydrogen reforming and the water shift reaction on-line. Pure hydrogen is removed from the reaction zone with a subsequent advantage to the reaction equilibrium.

Keywords: Membranes

398. **MICROSCOPIC AND MICROSTRUCTURAL ISSUES FOR OPTIMAL MATERIAL DESIGN**
$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
University of California at San Diego Contact: B. K. Kad (619) 534-7059

The objective of this work is to explore experimental and computational means by which inherent material and processing-induced anisotropies of ODS Fe_3Al-base alloys can be exploited to meet in-service mechanical and creep-life requirements of the power generation industry. The research shall examine microscopic and microstructural issues with a view to addressing optimum material design for macroscopic components under well prescribed in-service loading criteria. The economic incentive is the low cost of Fe_3Al-based alloys and its superior sulfidation resistance, in comparison to the competing Fe-Cr-Al base alloys and the Ni-base superalloys currently in service.

The development of suitable ODS Fe_3Al materials and processes shall endeavor to achieve high mechanical strength at temperature, as well as prolonged creep-life in service. Post-deformation recrystallization or zone annealing processes shall be examined as necessary to increase the grain size and to modify the grain shape for the anticipated use.

Keywords: Alloys

399. **FATIGUE AND FRACTURE BEHAVIOR OF Cr-X ALLOYS**
$75,000
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
University of Tennessee Contact: P. K. Liaw
(865) 974-6356

The objective of this research is to characterize the fatigue and fracture behavior of Cr_2Nb-based alloys and other intermetallic materials at ambient and elevated temperatures in controlled environments. These studies are expected to lead to mechanistic understanding of the fatigue and fracture behavior of these alloys. Fatigue tests are conducted for the purpose of evaluating crack initiation and fatigue life of Cr_2Nb-based alloys as well as other intermetallic alloys.

Keywords: Alloys

ULTRA-SUPERCRITICAL STEAM POWER PLANT RESEARCH

400. **ULTRA-SUPERCRITICAL STEAM TURBINE MATERIALS**
$200,000
DOE Contacts: F. M. Glaser (301) 903-2784,
V. U. S. Rao (412) 386-4743, M. H. Rawlins
(865) 576-4507
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: Materials, Power Plants, Turbines

401. **MATERIALS FOR ULTRA-SUPERCRITICAL STEAM POWER PLANTS**
$0
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

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: Materials, Power Plants

402. **ULTRA-SUPERCRITICAL STEAM CYCLE TURBINE MATERIALS**
$350,000
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

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: Materials, Power Plants, Turbines

VISION 21 SUPPORT ACTIVITIES

403. **IMPROVED ODS ALLOY FOR HEAT EXCHANGER TUBING**
$105,999
DOE Contacts: F. M. Glaser, (301) 903-2784 and R. B. Read (412) 386-5721
Special Metals Contact: M.A. Harper (304) 526-5057

Certain key components have been indentified as necessary for the success of a Vision 21 power plant, one of which is a high temperature heat exchanger. The project is to develop/produce an oxide dispersion strengthened (ODS) heat exchanger tube such that a full scale heat exchanger can be manufactured, and the alloy MA956 has been chosen for the material in this study. The main limitations of current ODS tubing are their poor weldability and relatively poor circumferential creep strength at elevated temperatures. Thus far, these two characteristics have restricted ODS materials to mostly non-pressure containing applications. Current conventional heat exchanger alloys have a maximum operating temperature of approximately 732˚C/1350˚F. Also, the maximum practical limit for current wrought Ni-base superalloys would be 860˚C/1580˚F. This Vision 21 project will use novel tube processing modifications to develop ODS tubes with sufficient strength for long term use at much higher temperatures (T>1093˚C/2000˚F). In addition, advanced welding techniques will be used to develop a joining method which will produce adequate joints on ODS materials. Thus the major tasks related to this objective are: (a) increasing the circumferential strength of a MA956 tube, (b) joining of the MA956 tube, and (c) determining the high temperature corrosion limits of the MA956 alloy in expected Vision 21 power plant environments.

Keywords: Oxide Dispersion Strengthened Alloys, Joining, Corrosion, Heat Exchanger, Vision 21

ADVANCED METALLURGICAL PROCESSES PROGRAM

The materials program at the Albany Research Center (ARC), formerly with the Bureau of Mines, 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 Vision 21 plants, 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 Richard Walters, (541) 967-5873.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

404. **ADVANCED FOIL LAMINATION TECHNOLOGY**
$560,000
DOE Contact: Richard P. Walters, (541) 967-5873
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

405. **ADVANCED CASTING TECHNOLOGIES**
$400,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact: Paul C. Turner (541) 967-5863

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

406. **ADVANCED REFRACTORIES FOR GASIFIERS**
$600,000
DOE Contact: Richard P. Walters (541) 967-5873
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 attach by molten coal slags in simulated gasifier environments has been developed.

Keywords: Refractories, Slagging Gasifier, Liners, Thermocouples

407. **OXIDATION AND SULFIDATION RESISTANT MATERIALS**
$600,000
DOE Contact: Richard P. Walters, (541) 967-5873
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

408. **WEAR AND ABRASION OF MATERIALS FOR FOSSIL ENERGY SYSTEMS**
$600,000
DOE Contact: Richard P. Walters (541) 967-5873
Albany Research Center Contact: Cindy Dogan (541) 967-5803

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

409. **MECHANISMS OF CORROSION UNDER ASH DEPOSITS**
$550,000
DOE Contact: Richard P. Walters, (541) 967-5873
Albany Research Center Contact: Cindy Dogan (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

410. **NON-ISOTHERMAL CORROSION AND OXIDATION**
$288,000
DOE Contact: Richard P. Walters, (541) 967-5873
Albany Research Center Contact: Cindy Dogan, (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

DIRECTORY

J. D. Achenbach
Department of Civil Engineering
Northwestern University
Evanston, IL 60201
(847) 491-5527

L. F. Allard
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(865) 574-4981

Richard Anderson
Kroftt-Brakston International, Inc.
5836 Sunrise Avenue
Claendon Hills, IL 60514
(708) 655-3207

P. Angelini
ORNL
P.O. Box 2008
Bldg. 4515, MS 6065
Oak Ridge, TN 37830-6065
(865) 574-4565

T. W. Arrigoni
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 972-4450

J. S. Arzigian
Division 1815
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2465

R. A. Assink
Division 1811
Sandia National Laboratories
Abuquerque, NM 87185
(505) 844-6372

D. G. Austin
9493 Dutch Hollow Road
Rixeyville, VA 22737
(540) 937-7953

V. Saimasarma Avva
N. Carolina State Univ.
Grahm Hall #8
Greensboro, NC 27411
(919) 379-7620

Walter C. Babcock
Bend Research, Inc.
64550 Research Road
Bend, OR 97701-8599
(503) 382-4100

Samuel J. Barish
ER-32/GTN
U.S. Dept. of Energy
19901 Germantown Road
Germantown, MD 20874-1290
(301) 903-3054

Lisa Barnett
EE-2K/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2212

Harold N. Barr
Hittman Mat. & Med. Components, Inc.
9190 Red Branch Road
Columbia, MD 21045
(301) 730-7800

Bulent Basol
Internl. Solar Electric Tech., Inc.
8635 Aviation Boulevard
Inglewood, CA 90301
(310) 216-4427

J. L. Bates
Pacific Northwest Laboratories
P.O. Box 999
Richland, WA 99352
(509) 375-2579

S. Bauer, Division G314
Sandia National Laboratory
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-9645

M. B. Beardsley
Caterpillar, Inc.
100 N.E. Adams Street
Peoria, IL 61629
(309) 578-8514

R. L. Beatty
ORNL
P.O. Box 2008
Bldg. 4508, MS 088
Oak Ridge, TN 37831
(865) 574-4536

P. F. Becher
ORNL
P.O. Box 2008
Bldg. 4515, 068, Room 275
Oak Ridge, TN 37831-6088
(865) 574-5157

David J. Beecy
FE-72/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-2787

Mohamad M. Behravesh
Nuclear Plant Corrosion Control
Electric Power Research Institute
3412 Hillview Avenue
Palo Alto, CA 94303
(650) 855-2388

William L. Bell
TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033
(303) 940-2301

John Benner
Solar Electric Conversion Div.
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 384-6496

Clifton G. Bergeron
University of Illinois
105 South Goodwin Avenue
204 Ceramics Building
Urbana, IL 61801
(217) 333-1770

Sam Berman
Bldg. 90, Rm. 3111
Lawerence Berkeley Laboratory
University of California
Berkeley, CA 94720
(510) 486-5682

Marita L. Berndt
Dept. of Energy Sciences & Technology
Brookhaven National Laboratory, Bldg. 526
Upton, NY 11973
(631) 344-3060

Theodore M. Besmann
Metals and Ceramics Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(865) 574-6852

Fritz Bien
Spectral Sciences, Inc.
99 South Bedford Street, #7
Burlington, MA 01803-5169
(617) 273-4770

J. Bockris
Texas A&M University
College Station, TX 77843-3255
(713) 845-5335

Robert Boettner
EE-112/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 252-9136

W. D. Bond
Oak Ridge National Laboratory
P.O. Box 2008
Bldg. 7920, 384, Room 0014
Oak Ridge, TN 37831-6088
(865) 574-7071

J. A. M. Boulet
University of Tennessee
310 Perkins Hall
Knoxville, TN 37996
(865) 974-8376

D. J. Bradley
Pacific Northwest National Laboratory
Richland, WA 99352
(509) 375-2587

R. A. Bradley
ORNL
P.O. Box 2008
Bldg. 4515
Oak Ridge, TN 37831-6067
(865) 574-6094

Joyce M. Brien
Research International, Inc.
18706-142nd Avenue, NE
Woodinville, WA 98072
(206) 486-7831

C. R. Brinkman
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 154
Oak Ridge, TN 37831
(865) 574-5106

Leslie Bromberg
Plasma Fusin Center
MA Institute of Tech.
Cambridge, MA 02139
(617) 253-6919

J. A. Brooks
Division 8312
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2051

Alexander Brown
Chesapeake Composites Corporation
239 Old Churchman's Road
New Castle, DE 19720
(302) 324-9110

Ian G. Brown
Lawrence Berkeley Laboratory
Berkeley, CA 94720
(510) 486-4147

S. T. Buljan
GTE Laboratories, Inc.
40 Sylvan Road
Waltham, MA 02254
(617) 890-8460

Kenneth R. Butcher
Selee Corporation
700 Shepherd Street
Hendersonville, NC 28792
(704) 697-2411

Oral Buyukozturk
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-7186

Elton Cairns
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(510) 486-5028

Juan Carbajo
ORNL
P.O. Box Y
Oak Ridge, TN 37831
(865) 574-3784

R. W. Carling, Div. 8313
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2206

P. T. Carlson
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(865) 574-5135

D. W. Carroll
LANL
Los Alamos, NM 87545
(505) 667-2145

Gloria M. Caton
ORNL
1060 Commerce Park
MS 6480
Oak Ridge, TN 37830
(865) 574-7759

Ken Chacey
EM-34/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-7186

A. T. Chapman
Georgia Institute of Technology
Georgia Tech Research Institute
Atlanta, GA 30332-0420
(404) 894-4815

Yok Chen
SC-131/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3428

Lalit Chhabildas
Org. 1433 Mail Stop 0821
P.O. Box 5800
Sandia National Laboratory
Albuquerque, NM 87185
(505) 844-4147

Richard Christensen
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 422-7136

L. Christophorou
ORNL
P.O. Box 2008
Bldg. 4500S, 122, Rm. H156
Oak Ridge, TN 37831
(865) 574-6199

Russel J. Churchill
American Research Corp. of Va.
642 First Street
P.O. Box 3406
Radford, VA 24143-3406
(703) 731-0836

M. J. Cieslak
MS 0887
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-0887
(505) 846-7500

D. E. Clark
Materials Technology Div
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
(208) 526-0746

S. K. Clark
Dept. of Mech. Eng. & App. Mech.
University of Michigan
Ann Arbor, MI 48109
(313) 764-4256

David Clarke
Univ. of California
Materials Department
Engineering III
Santa Barbara, CA 93106
(805) 893-8275

R. L. Clough
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-3492

Joe K. Cochran, Jr.
School of Ceramic Eng.
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-2851

Robert Cook
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 422-6993

Alastair N. Cormack
NYS College of Ceramics
Alfred University
Alfred, NY 14802
(607) 871-2180

J. E. Costa
Division 8314
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2352

James V. Crivello
Department of Chemistry
Rensselaer Polytechnic Institute
Troy, NY 12180-3590
(518) 276-6825

Randy Curlee
ORNL
P.O. Box 2008
Oak Ridge, TN 37831
(865) 576-4864

David I. Curtis
NR-1 Bldg. 104
U.S. Dept of Energy
Washington, DC 20585
(202) 781-6141

G. J. D'Alessio
DP-242/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-6688

S. J. Dapkunas
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 975-6119

John Davis
McDonnell Douglas Astro. Co.
Fusion Energy Program
P.O. Box 516, Bldg 278
St. Louis, MO 63166
(314) 234-4826

Robert F. Davis
Dept. of Materials Eng.
North Carolina State University
232 Riddick Lab, Box 7907
Raleigh, NC 27695
(919) 737-3272

Victor Der
ER-531/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5736

R. Diegle
Division 1841
Sandia National Labs
Albuquerque, NM 87185
(505) 846-3450

R. Diercks
Mat. Science & Tech. Div.
Argonne National Labs
9700 South Cass Ave
Argonne, Illinois 60439
(630) 972-5032

Larry A. Dominey
Covalent Associates, Inc.
10 State Street
Woburn, MA 01801
(617) 938-1140

Elaine Drew
Supercon, Inc.
830 Boston Turnpike
Shrewsbury, MA 01545
(508) 842-0174

C. Duffy
LANL P.O. Box 1663
Los Alamos, NM 87545
(505) 843-5154

E. M. Dunn
GTE Laboratories, Inc.
40 Sylvan Road
Waltham, MA 02254
(617) 466-2312

Sunil Dutta
NASA Lewis Research Center
21000 Brookpark Road, MS 49-3
Cleveland, OH 44135
(216) 433-3282

Christopher A. Ebel
Norton Company
Goddard Road
Northboro, MA 01532-1545
(617) 393-5950

James J. Eberhardt
EE-2G/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9837

G. R. Edwards
Colorado School of Mines
Golden, CO 80401
(303) 273-3773

Paul Eggerstedt
Ind. Filter & Pump Man. Co.
5900 Ogden Avenue
Cicero, IL 60650
(708) 656-7800

W. A. Ellingson
Argonne National Laboratories
Mat. Science Div., Bldg. 212
9700 South Cass
Argonne, Illinois 60439
(630) 252-5068

Gerald Entine
Radiation Monitoring Devices, Inc.
44 Hunt Street
Watertown, MA 02172
(617) 926-1167

Mike Epstein
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-6424

John Fairbanks
EE-2G/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8066

P. D. Fairchild
ORNL
P.O. Box Y
Bldg. 9102-2, 001, Room 0210
Oak Ridge, TN 37831
(865) 574-2009

D. A. Farkas
Virginia Polytechnic Institute
and University
Mat. Sci. and Eng.
201 A Holden Hall
Blacksburg, VA 24061
(540) 231-4742

Cynthia K. Farrar
Montec Associates, Inc.
P.O. Box 4182
Butte, MT 59702
(406) 494-2596

W. Feduska
Westinghouse Electric Corp.
R&D Center
1310 Beulah Road
Pittsburgh, PA 15235
(412) 256-1951

Robert S. Feigelson
Center for Materials Research
Stanford University
Stanford, CA 94305
(650) 723-4007

Mattison K. Ferber
ORNL
P.O. Box 2008
Building 4515
Oak Ridge, TN 37831-6064
(865) 576-0818

Nicholas Fiore
Carpenter Technology Corp.
101 West Bern Street
P.O. Box 14662
Reading, PA 19612
(215) 371-2556

Ronald J. Fiskum
EE-422/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9130

D. M. Follstaedt
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2102

Christopher A. Foster
Cryogenic Applications F, Inc.
450 Bacon Springs Lane
Clinton, TN 37716
(865) 435-5433

Mark Frei
EM-34/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-7201

Ehr-Ping Huang Fu
Thermal Science
EE-2F/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1493

P. W. Fuerschbach
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-2464

E. R. Fuller
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2942

F. D. Gac
LANL/MS G771
Los Alamos, NM 87545
(505) 667-5126

G. F. Gallegos
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 422-7002

F. P. Gerstle, Jr.
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-4304

C. P. Gertz
Yucca Mountain Project Mgr.
U.S. Dept. of Energy
P.O. Box 98518
Las Vegas, NV 89193
(702) 794-7920

Larry Gestaut
Eltech Systems Corp.
Painsville, OH 44077
(216) 357-4041

R. Glass
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 423-7140

Leon Glicksman
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-2233

Martin Glicksman
Rensselear Polytechnic Inst.
Materials Research Ctr. - 104
8th Street
Troy, NY 12180-3690
(518) 276-6721

Robert L. Goldsmith
CeraMem Corporation
12 Clematis Avenue
Waltham, MA 02154
(617) 899-0467

B. Goodman
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-1005

S. H. Goods
Divison 8314
Sandia National Laboratories
Livermore, CA 94550
(925) 422-3274

R. J. Gottschall
ER-13/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3427

Anton C. Greenwald
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

N. Grossman
NE-42/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3745

Dieter M. Gruen
Materials Science Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(630) 252-3513

Adi R. Guzdar
Foster-Miller, Inc.
350 Second Avenue
Waltham, MA 02154
(617) 890-3200

John P. Gyeknyesi
NASA Lewis Research Center
2100 Brookpark Road, MS 49-7
Cleveland, OH 44135
(216) 433-3210

J. S. Haggarty
MIT
77 Massachussetts Avenue
Cambridge, MA 02139
(617) 253-2129

Phil Haley
Allison Turbine Operations
P.O. Box 420
Indianapolis, IN 46206-0420
(317) 230-2272

David G. Hamblen
Advanced Fuel Research, Inc.
87 Church Street
P.O. Box 380379
East Hartford, CT 06138-0379
(203) 528-9806

Edward P. Hamilton
American Superconductor Corp.
2 Technology Drive
Westboro, MA 01581
(508) 836-4200

Debbie Haught
EE-2D/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2211

Jeff Hay
Chem.-Mat. Science Div.
Los Alamos National Lab
Los Alamos, NM 87545
(505) 843-2097

Norman L. Hecht
University of Dayton
300 College Park, KL165
Dayton, OH 45469-0001
(513) 229-4343

Kamithi Hemachalam
Intermagnetics General Corp.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Mary T. Hendricks
Alabama Cryogenic Engineering, Inc.
P.O. Box 2470
Huntsville, AL 35804
(205) 536-8629

Carolyn J. Henkens
Andcare, Inc.
2810 Meridian Parkway
Suite 152
Durham, NC 27713
(919) 544-8220

Carl Henning
Lawrence Livermore Nat. Lab
P.O. Box 5511
Livermore, CA 94550
(925) 532-0235

G. Duncan Hitchens
Lynntech, Inc.
7610 Eastmark Drive
Suite 105
College Station, TX 77840
(409) 693-0017

Kai-Ming Ho
Inst. for Physical
Research and Technology
Ames Laboratory
Ames, IA 50011
(515) 294-1960

J. M. Hobday
METC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4347

D. M. Hoffman
Lawrence Livermore Nat. Lab
University of California
P.O. Box 808
Livermore, CA 94550
(510) 422-7759

E. E. Hoffman
U.S. Dept. of Energy
P.O. Box 2001
Oak Ridge, TN 37831-8600
(865) 576-0735

Linda L. Horton
Oak Ridge National Laboratory
Box 2008, Bldg. 4500-S
Oak Ridge, TN 37831-6118
(865) 574-5081

E. Philip Horwitz
Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(630) 252-3653

Stephen M. Hsu
Center for Materials Science
National Measurements Lab
NIST
Gaithersburg, MD 20899
(301) 975-6119

Donald R. Huffman
Dept. of Physics
University of Arizona
Tucson, AZ 85721
(520) 621-4804

Arlon Hunt
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(925) 486-5370

George F. Hurley
Chemistry-Materials Sci. Div.
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-9498

Mallika D. Ilindra
Sumi Tech, Inc.
3006 McLean Court
Blacksburg, VA 24060
(540) 552-8334

D. David Ingram
Universal Energy Systems, Inc.
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

L. K. Ives
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-2843

David A. Jackson
Energy Photovoltaics, Inc.
276 Bakers Basin Road
Lawrenceville, NJ 08648
(609) 587-3000

Jonah Jacob
Science Research Lab, Inc.
15 Ward Street
Somerville, MA 02143
(617) 547-1122

N. S. Jacobson
NASA Lewis Research Center
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-5498

Radha Jalan
ElectroChem, Inc.
400 West Cummings Park
Woburn, MA 01801
(617) 932-3383

Mark A. Janney
ORNL
P.O. Box 2008
Bldg. 4515, 069, Room 228
Oak Ridge, TN 37831-6088
(865) 574-4281

J. E. Jensen
CVI Inc.
P.O. Box 2138
Columbus, OH 43216
(614) 876-7381

Carl E. Johnson
Chemical Technology Division
Argonne National Laboratory
9700 Cass Ave, Bldg. 205
Argonne, IL 60439
(630) 252-7609

Curtis A. Johnson
GE Research Laboratory
P.O. Box 8
Bldg. 31 #3C7
Schenectady, NY 12301
(518) 387-6421

D. Ray Johnson
ORNL, Metals & Ceramics Div.
P.O. Box 2008
Bldg. 4515, 066, Room 206
Oak Ridge, TN 37831-6088
(865) 576-6832

Robert Jones
Los Alamos National Lab.
P.O. Box 1663, M/S J577
Los Alamos, NM 87545
(505) 667-6441

Robert A. Jones
DP-28/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-4236

Landis Kannberg
Pacific Northwest Lab
Battlelle Blvd.
P.O. Box 999
Richland, WA 99352
(509) 375-3919

Michael E. Karpuk
TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033
(303) 940-2301

M. E. Kassner
Oregon State University
Dept. Of Mechanical Engineering
Rogers 204
Corvallis, OR 97331-5001
(541) 737-7023

Carlos Katz
Cable Technology Lab
P.O. Box 707
New Brunswick, NJ 08903
(201) 846-3220

Joel Katz
LANL
P.O. Box 1663/MS G771
Los Alamos, NM 87545
(505) 665-1424

Robert N. Katz
Worcester Polytechnical Inst.
Dept. of Mechanical Eng.
100 Institute Street
Worcester, MA 01609
(508) 831-5336

Larry Kazmerski
Solar Electric Conv. Div.
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 384-6600

M. R. Keenan
Division 1813
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6631

J. R. Keiser
ORNL
P.O. Box 2008
Bldg. 4500-S, 156, Room 0734
Oak Ridge, TN 37830
(865) 574-4453

Rudolf Keller
EMEC Consultants
4221 Roundtop Road
Export, PA 15632
(412) 325-3260

Han Kim
GTE Labs
40 Sylvan Road
Waltham, MA 02254
(617) 466-2742

Christopher N. King
Planar Systems, Inc.
1400 Northwest Compton Drive
Beaverton, OR 97006
(503) 690-1100

Richard King
EE-2A/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1693

J. H. Kinney
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 422-6669

G. S. Kino
Edward Ginzton Laboratory
Stanford University
Stanford, CA 94305
(925) 497-0205

Paul Klemmens
University of Connecticut
Box U-46
Storrs, CT 06268
(860) 486-3134

S. J. Klima
NASA Lewis Research Center
MS 106-1
21000 Brookpark Road
Cleveland, OH 44135
(216) 433-6020

J. A. Knapp
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-2305

G. A. Knorovsky
Division 1833
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1109

Timothy R. Knowles
Energy Science Labs, Inc.
6888 Nancy Ridge Drive
San Diego, CA 92121-2232
(619) 552-2034

Victor R. Koch
Covalent Associates, Inc.
10 State Street
Woburn, MA 01801
(617) 938-1140

Dale Koelling
SC-13/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-2187

K. G. Kreider
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 975-2619

David Kurtz
Advanced Technology Materials, Inc.
7 Commerce Drive
Danbury, CT 06810
(203) 794-1100

S. R. Kurtz
Division 1811
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5436

Richard J. Lagow
Department of Chemistry
The Univ. of Texas at Austin
Austin, TX 78712
(512) 471-1032

James Lankford
Southwest Research Inst.
6220 Culebra Road
P.O. Drawer 28510
San Antonio, TX 78284
(512) 684-5111

R. LaSala
EE-2C/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4198

W. N. Lawless
CeramPhysics, Inc.
921 Eastwind Drive, Suite 110
Westerville, OH 43081
(614) 882-2231

S. R. Lee
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 675-6137

Franklin D. Lemkey
United Tech. Research Ctr.
Silver Lane
East Hartford, CT 06108
(860) 727-7318

Douglas Lemon
Pacific Northwest Labs
P.O. Box 999
Richland, WA 99352
(509) 375-2306

S. R. Levine
NASA Lewis Research Center
21000 Brookpart Road
Cleveland, OH 44135
(216) 433-3276

C. T. Liu, Mtl. Ceram. Div.
ORNL
P.O. Box 2008
Bldg. 4500-S, 115, Rm. S280
Oak Ridge, TN 37831
(865) 574-5516

K. C. Liu
ORNL
P.O. Box 2008
Bldg. 4500-S, MS 155
Oak Ridge, TN 37831
(865) 574-5116

Richard W. Longsderff
Thermacore, Inc.
780 Eden Road
Lancaster, PA 17601
(717) 569-6551

R. O. Loutfy
Mat. & Electro. Research Corp.
7960 South Kolb Road
Tucson, AZ 85706
(602) 574-1980

T. C. Lowe
Divison 8316
Sandia National Laboratories
Livermore, CA 94550
(925) 422-3187

C. D. Lundin
307 Dougherty Eng. Bldg.
University of Tennessee
Knoxville, TN 37996
(865) 974-5310

MAJ Ross E. Lushbough
DP-225.2/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3912

Richard Mah
Los Alamos National Lab
P.O. Box 1663
Los Alamos, NM 87545
(505) 607-3238

Mokhtas S. Maklad
EOTEC Corporation
420 Frontage Road
West Haven, CT 06516
(203) 934-7961

Frederick M. Mako
FM Technologies
4431-H Brookfield Corporate Drive
Chantilly, VA 20151
(703) 961-1051

A. C. Makrides
EIC Laboratories, Inc.
111 Downey Street
Norwood, MA 02062
(617) 769-9450

Mark K. Malmros
MKM Research/Ohmicron
P.O. Box I
Washington Crossing, PA 18977
(609) 737-9050

Matthew Marrocco
Maxdem, Inc.
140 East Arrow Highway
San Dimas, CA 91773
(909) 394-0644

R. G. Martin
Analysis Consultants
21831 Zuni Drive
El Toro, CA 92630
(714) 380-1204

H. Maru
Energy Research Corporation
3 Great Pasture Road
Danbury, CT 06810
(203) 792-1460

K. Masubuchi
Lab for Manuf. and Prod.
MIT
Cambridge, MA 02139
(617) 255-6820

Ronald D. Matthews
Dept. of Mechanical Engineering
The University of Texas at Austin
Austin, TX 78712
(512) 471-3108

Douglas McAllister
BIODE, Inc.
2 Oakwood Road
Cape Elizabeth, ME 04107
(207) 883-1492

D. McCright
LLNL
University of California
Livermore, CA 94550
(213) 423-7051

Patrick N. McDonnell
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

David L. McElroy
ORNL
P.O. Box 2008
Bldg. 4508, 092, Rm. 239
Oak Ridge, TN 37831-6088
(865) 574-5976

A. J. McEvily
Metallurgy Dept., U-136
University of Connecticut
Storas, CT 06268
(860) 486-2941

T. D. McGee
Mat. Science & Engineering
110 Engineering Annex
Iowa State University
Ames, IA 50011
(515) 294-9619

Carl McHargue
University of Tennessee
Materials & Eng. Dept.
434 Doughtery Eng. Bldg.
Knoxville, TN 37996-2200
(865) 974-8013

Arthur S. Mehner
NE-53/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-4474

G. H. Meier
848 Benevum Hall
University of Pittsburgh
Pittsburgh, PA 15261
(412) 624-5316

A. Meyer
International Fuel Cells
P.O. Box 739
195 Governors Hwy.
South Windsor, CT 06074
(203) 727-2214

JoAnn Milliken
EE-2H/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2480

B. E. Mills
Sandia National Laboratories
Livermore, CA 94550
(925) 422-3230

Andrew Morrison
M/S 238-343
Flat Plate Solar Array Project
Jet Propulsion Laboratory
Pasadena, CA 91109
(213) 354-7200

Craig Mortenson
BPA/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-5656

J. Moteff
University of Cincinnati
Department of Material Science
Metallurgical Engineering
498 Rhodes Hall
Cincinnati, OH 45221-0012
(513) 475-3096

Leszek R. Motowidlo
IGC Advanced Superconductors
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Arnulf Muan
Pennsylvania State University
EMS Experiment Station
415 Walker Bldg.
University Park, PA 16802
(814) 865-7659

L. Marty Murphy
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 231-1050

J. Narayan
Materials Science & Eng.
North Carolina State Univ.
Box 7916
Raleigh, NC 27695-7916
(919) 515-7874

Michael Nastasi
Los Alamos National Lab
Los Alamos, NM 87545
(505) 667-7007

K. Natesan
Argonne National Lab.
Materials Science Division
9700 South Cass
Argonne, IL 60439
(630) 252-5103

M. Naylor
Cummins Engine Co., Inc.
Box 3005
Mail Code 50183
Columbus, IN 47202-3005
(812) 377-5000

M. C. Nichols
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2906

P. J. Nigrey
Division 1150
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8985

D. A. Nissen
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2767

T. A. Nolan
ORNL
P.O. Box 2008
Bldg. 4515, MS 064
Oak Ridge, TN 37831
(865) 574-0811

Paul C. Nordine
Containerless Research, Inc.
910 University Place
Evanston, IL 60201-3149
(708) 467-2678

P. C. Odegard
Divison 8216
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2789

G. R. Odette
Dept. of Chem. & Nuclear Eng.
University of California
Santa Barbara, CA 93106
(805) 961-3525

Thomas Ohlemiller
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-3771

Ben Oliver
Materials Science & Eng.
421 Dougherty Hall
Knoxville, TN 37996
(865) 974-5326

G. C. Osbourn
Division 1130
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-8850

Roland Otto
Lawrence Berkeley Lab.
Bldg 73, 106A
Berkeley, CA 94720
(510) 486-5289

G. M. Ozeryansky
IGC Superconductors, Inc.
1875 Thomaston Avenue
Waterbury, CT 06704
(203) 753-5215

Richard H. Pantell
Electrical Engineering Dept.
Stanford University
Stanford, CA 94305
(650) 723-2564

E. R. Parker
456 Hearst
Univ. of Ca., Berkeley
Berkeley, CA 24720
(510) 642-0863

Bill Parks
EE-2D/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2093

D. O. Patten
Norton Company
High Performance Ceramics
Goddard Road
Northboro, MA 01532
(617) 393-5963

Ahmad Pesaran
NREL
1617 Cole Blvd.
Golden, CO 80401
(303) 231-7636

John Petrovic
Chemistry-Mat. Science Div.
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-5452

S. T. Picraux
Division 1110
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-7681

R. D. Pierce
Argonne National Laboratories
Chemical Tech Division
Bldg. 205, Room W-125
Argonne, IL 60439
(630) 972-4450

Melvin A. Piestrup
Adelphi Technology
13800 Skyline Blvd.
Woodside, CA 94062
(925) 851-0633

Joseph Prahl
Case Western Reserve Univ.
Cleveland, OH 44106
(216) 368-2000

Mark A. Prelas
Nuclear Engineering Program
University of Missouri
Columbia, MO 65211
(314) 882-3550

Peter Pronko
Universal Energy Systems
4401 Dayton-Xenia Road
Dayton, OH 45432
(513) 426-6900

Herschel Rabitz
Dept. of Chemistry
Princeton University
Princeton, NJ 08544-1009
(609) 258-3917

Robert Rapp
Dept. of Metal. Eng.
Ohio State University
Columbus, OH 43210
(614) 422-2491

Bhakta B. Rath, Assoc. Dir. Res.
Naval Research Laboratory
Mat. Science & Component Tech.
Building 43, Room 212 - Code 6000
Washington, DC 20375-5000
(202) 767-3566

Rod Ray
Bend Research, Inc.
64550 Research Road
Bend, OR 97701-8599
(503) 382-4100

Brian Rennex
Natl. Institute of Standards
and Technology
Center of Bldg. Technology
Gaithersburg, MD 20899
(301) 921-3195

S. Richlen
EE-2F/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-2078

R. O. Ritchie
456 Hearst
University of Cal., Berkeley
Berkeley, CA 24720
(510) 642-0863

R. B. Roberto
ORNL
Solid State Division
P.O. Box 2008
Oak Ridge, TN 37831-6030
(865) 574-6151

D. I. Roberts
GA Technologies
P.O. Box 81608
San Diego, CA 92138
(619) 455-2560

S. L. Robinson
Division 8314
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2209

Timothy L. Rose
EIC Laboratories, Inc.
111 Downing Street
Norwood, MA 02062
(617) 764-9450

John H. Rosenfeld
Thermacore, Inc.
780 Eden Road
Lancaster, PA 17601
(717) 569-6551

P. N. Ross
Mat. & Metal. Research Div.
Lawrence Berkeley Labs
University of Berkeley
Berkeley, CA 94720
(510) 486-4000

Giulio A. Rossi
Norton Company
Goddard Road
Northboro, MA 01532-1545
(617) 393-5829

Walter Rossiter
Center for Bldg. Technology
National Institute of Standards
and Technology
Gaithersburg, MD 20899
(301) 921-3109

M. Rubin
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
(510) 486-7124

E. Russell
LLNL
University of California
Livermore, CA 94550
(925) 423-6398

C. O. Ruud
159 MRL
University Park, PA 16802
(814) 863-2843

John Ryan
EE-2J/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8823

Djordjiji R. Sain
Nuclear Con. Services, Inc.
P.O. Box 29151
Columbus, OH 43229
(614) 846-5710

R. J. Salzbrenner
Division 1832
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-5041

Stuart Samuelson
Deltronic Crystal Industries, Inc.
60 Harding Avenue
Dover, NJ 07801
(201) 361-2222

J. Sankar
Dept of Mechanical Engineering
North Carolina A&T University
Greensboro, NC 27411
(919) 379-7620

Mike L. Santella
ORNL
P.O. Box 2008
Oak Ridge, TN 37831-6088
(865) 574-4805

Srinivasan Sarangapani
ICET, Inc.
916 Pleasant Street
Unit 12
Norwood, MA 02062
(617) 679-6064

V. K. Sarin
GTE
40 Sylvan Road
Waltham, MA 02254
(617) 890-8460

Suri A. Sastri
Surmet Corporation
33 B Street
Burlington, MA 01803
(617) 272-3250

Jerome J. Schmidt
Jet Process Corporation
25 Science Park
New Haven, CT 06511
(203) 786-5130

Erland M. Schulson
33 Haskins Road
Hanover, NH 03755
(603) 646-2888

James Schwarz
Dept. Chem. Eng/Mat Science
Syracuse University
320 Hinds Hall
Syracuse, NY 13244
(315) 423-4575

James L. Scott
Metals and Ceramics Div.
ORNL
P.O. Box 2008, Bldg. 4508
Oak Ridge, TN 37831-6091
(865) 624-4834

Timothy C. Scott
Chemical Technology Division
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831
(865) 574-5962

R. E. Setchell
Division 1130
Sandia National Labs
Albuquerque, NM 87185
(505) 844-5459

Suzanne C. Shea
Praxis Engineers, Inc.
852 North Hillview Drive
Milpitas, CA 95035
(408) 945-4282

D. E. Shelor
RW-3/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9433

V. K. Sikka
ORNL
P.O. Box 2008
Bldg. 4508, 083, Rm. 129
Oak Ridge, TN 37831
(865) 574-5112

Richard Silberglitt
RAND
1200 South Hayes Street
Arlington, VA 22202
(703) 413-1100 x5441

T. B. Simpson
FE-34/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3913

J. P. Singh
Argonne National Labs
9700 South Cass
Argonne, IL 60439
(630) 252-5123

Maurice J. Sinnott
Chemical and Metall. Eng.
University of Michigan
H Dow Building
Ann Arbor, MI 48109-2136
(313) 764-4314

Piran Sioshamsi
Spire Corporation
Patriots Park
Bedford, MA 02173
(617) 275-6000

Kurt D. Sisson
EE-222/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-6750

Jerry Smith
SC-132/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3426

M. F. Smith
Division 1834
Sandia National Laboratories
Albuquerque, NM 87185
(505) 846-4270

Peter L. Smith
Newton Optical Technologies
167 Valentine Street
Newton, MA 02165
(617) 495-4984

J. E. Smugeresky
Division 8312
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2910

Mike Soboroff
IMF Program
EE-2F/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-4936

N. R. Sorensen
Division 1841
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-1097

Charles A. Sorrell
EE-2F/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1514

R. F. Sperlein
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 972-5985

J. R. Springarn
Division 8312, SNL
Livermore, CA 94550
(925) 422-3307

Mark B. Spitzer
Spire Corporation
Patriots Park
Bedford, MA 01730
(617) 275-6000

T. L. Starr
Georgia Tech Res. Inst.
Georgia Inst. of Technology
Atlanta, GA 30332
(404) 894-3678

Wayne S. Steffier
Hyper-Therm, Inc.
18411 Gothard Street
Units B & C
Huntington Beach, CA 92648
(714) 375-4085

Helmut F. Stern
Arcanum Corporation
P.O. Box 1482
Ann Arbor, MI 48106
(313) 665-4421

George Stickford
Battelle-Columbus Labs
505 King Avenue
Columbus, OH 43201
(614) 424-4810

Thomas J. Stiner
AstroPower, Inc.
Solar Park
Newark, DE 19716
(302) 366-0400

D. P. Stinton
ORNL
P.O. Box 2008
Bldg. 4515, 063, Rm. 111
Oak Ridge, TN 37831
(865) 574-4556

Norman Stoloff
Materials Engineering Dept.
Rensselaer Polytechnic Inst.
Troy, NY 12181
(518) 266-6436

Paul D. Stone
The Dow Chemical Company
1776 Eye Street, NW, #575
Washington, DC 20006

J. E. Stoneking
Dept. of Eng. Science & Mech.
310 Perkins Hall
Knoxville, TN 37996
(865) 974-2171

David Sutter
ER-224/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-5228

Richard Swanson
SunPower Corporation
435 Indio Way
Sunnyvale, CA 94086
(408) 991-0900

R. W. Swindeman
ORNL
P.O. Box 2008
Bldg. 4500-S, 155, Rm. 0040
Oak Ridge, TN 37831
(865) 574-5108

W. Tabakoff
Dept. of Aerospace Eng.
M/L 70
University of Cincinnati
Cincinnati, OH 45221
(513) 475-2849

C. A. Thomas
U.S. Dept. of Energy
P.O. Box 10940
Pittsburgh, PA 15236
(412) 972-5731

Iran L. Thomas
ER-10/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-3426

D. O. Thompson
Ames Laboratory
Iowa State University
Ames, IA 50011
(515) 294-5320

T. Y. Tien
Mat. and Metal. Eng.
University of Michigan
Ann Arbor, MI 48109
(813) 764-9449

T. N. Tiegs
ORNL
Bldg. 4515, 069, Rm. 230
P.O. Box 2008
Oak Ridge, TN 37831-6088
(865) 574-5173

Jyh-Ming Ting
Applied Sciences, Inc.
141 West Xenia Avenue
P.O. Box 579
Cedarville, OH 45314
(513) 766-2020

R. H. Titran
NASA Lewis Research Center
21000 Brookpark Road, MS 49-1
Cleveland, OH 44135
(216) 433-3198

Zygmunt Tomczuk
Chemical Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
(708) 252-7294

Micha Tomkiewicz
Physics Department
Brooklyn College of City
University of New York
Brooklyn, NY 11210
(718) 951-5357

John J. Tomlinson
ORNL
Bldg. 9204-1, MS 8045
P.O. Box 2009
Oak Ridge, TN 37831-8045
(865) 574-0768

Carl R. Vander Linden
Vander Linden & Associates
AIC Materials Program
5 Brassie Way
Littleton, CO 80123
(303) 794-8309

Richard D. Varjian
Dow Chemical Company, Inc.
Central Research - Catalysis
1776 Building
Midland, MI 49675
(517) 636-6557

Matesh Varma
SC-13/GTN
U.S. Dept. of Energy
19901 Germantown Road
Germantown, MD 20874-1290
(301) 903-3209

Krishna Vedula
Dept. of Metal. & Mat. Science
Case Western Reserve University
10900 Euclid Avenue
Cleveland, OH 44115
(216) 368-4211

Robert W. Vukusich
UES, Inc.
4401 Dayton-Xenia Road
Dayton, OH 45432-1894
(513) 426-6900

J. B. Walter
Materials Technology Div.
Idaho National Eng. Lab
Idaho Falls, ID 83415
(208) 526-2627

John Walter
IntraSpec, Inc.
P.O. Box 4579
Oak Ridge, TN 37831
(865) 483-1859

William K. Warburton
X-ray Instrumentation Associates
1300 Mills Street
Menlo Park, CA 94025-3210
(925) 903-9980

Craig N. Ward
Ultramet
12173 Montague Street
Pacoima, CA 91331
(818) 899-0236

Gary S. Was
Dept. of Nuclear Eng.
University of Michigan
Ann Arbor, MI 48109
(313) 763-4675

Rolf Weil
Dep. of Mat. & Metal. Eng.
Stevens Inst. of Technology
Castle Point Station
Hoboken, NJ 07030
(201) 420-5257

Roy Weinstein
Instit. for Particle Beam Dynamics
University of Houston
Houston, TX 77204-5502
(713) 743-3600

Elizabeth G. Weiss
Membrane Technology and Research, Inc.
1360 Willow Road, Suite 103
Menlo Park, CA 94025
(925) 328-2228

James Wert
Mech. Eng. Dept.
Vanderbilt University
Station B, P.O. Box 1592
Nashville, TN 37235
(615) 322-2413

Sheldon M. Wiederhorn
National Institute of Standards
and Technology
Bldg. 223, #A329
Gaithersburg, MD 20899
(301) 975-2000

Daniel E. Wiley
Dir. of Improved Energy Prod.
EE-231/FORS
U.S. Dept. of Energy
Washington, DC 2085
(202) 586-2099

Frank Wilkins
EE-2A/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-1684

A. D. Wilks
Signal UOP Research Center
50 UOP Plaza
Des Plaines, IL 60016
(312) 492-3179

Lane Wilson
National Energy Tech Lab (NETL-MGN)
Gas Power Projects Division
3610 Collins Ferry Road
Morgantown, WV 26507-0880
(304) 285-1336

C. E. Witherell
LLNL
University of California
P.O. Box 808
Livermore, CA 94550
(925) 422-8341

J. C. Withers
Mat. & Electro. Res. Corp.
7960 South Kolb Road
Tucson, AZ 85706
(602) 574-1980

D. E. Wittmer
S. Illinois Univ./Carbondale
Dept. of Mech. Eng. & Egy Pro.
Carbondale, IL 62901
(618) 536-2396, ext. 21

T. Wolery
LLNL
University of California
Livermore, CA 94550
(925) 423-5789

Stanley M. Wolf
EM-54/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-7962

J. R. Wooten
Rocketdyne
6633 Canoga Avenue
Mail Code BA-26
Canoga Park, CA 91303
(818) 710-5972

John D. Wright
TDA Research, Inc.
12345 West 52nd Avenue
Wheat Ridge, CO 80033
(303) 940-2301

R. N. Wright
Materials Technology Div.
Idaho National Eng. Laboratory
Idaho Falls, ID 83415
(208) 526-6127

Thomas M. Yonushonis
Cummins Engine Co., Inc.
Box 3005
Mail Code 50183
Columbus, IN 47202-3005
(812) 377-7078

J. Yow
LLNL
University of California
Livermore, CA 94550
(925) 423-3521

Dingan Yu
Supercon, Inc.
830 Boston Turnpike
Shrewsbury, MA 01545
(508) 842-0174

Charlie Yust
ORNL
P.O. Box 2008
Bldg. 4515, 063, Rm. 106
Oak Ridge, TN 37830
(865) 574-4812

C. M. Zeh
FETC
P.O. Box 880
Morgantown, WV 26505
(304) 291-4265

Kenneth Zwiebel
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 384-6441

APPENDIX

Department of Energy
Washington, DC 20585

MEMORANDUM FOR RAYMOND L. ORBACH
DIRECTOR
OFFICE OF SCIENCE

FROM: DALE D. KOELLING
CHAIR, ENERGY MATERIALS COORDINATING
COMMITTEE (EMaCC)

SUBJECT: Request for Approval of Minor Revision of the EMaCC Charter.

I request your approval of some minor revisions of the EMaCC Charter, which was approved in 1993, principally to incorporate provisions for document storage.

The EMaCC embraces 19 program offices across DOE that have various responsibilities for materials research or development. It provides a formal structure for communication and coordination between these offices. A report is published annually. EMaCC reports to the Director, Office of Science.

The major problem addressed by this revision is the archiving of documents. Previously. documents were retained by the EMaCC officers and passed along with each annual change of management. This system, being no stronger than the weakest link in the chain of offices, has failed. To permanently remedy this, the revised Charter calls for the Division of Materials Science and Engineering in the Office of Basic Energy Sciences to provide a computerized repository. One other substantive change has been made: to remove the early prohibition from considering biological constructs. This reflects the fact that biological systems are now being used in the development of new materials. The remaining changes are important but not substantive. The final change in the new Charter is to change its name from "Terms of Reference" to "Charter."

Attachment: Proposed revised Charter for the Energy Materials Coordinating Committee

Approve: ______________

Disapprove: ______________

Date: JUN 0 5 2003

EMaCC Charter Memo

04/18/03

CHARTER FOR THE DOE
ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

The DOE Energy Materials Coordinating Committee (EMaCC) is a working group reporting to the Director of the Office of Science in the materials research and development aspects of the Director's statutory role (42 USC 7139b2 et seq.) as advisor to the Secretary of Energy in monitoring the Department's energy research and development program.

The purpose of the EMaCC is to:

(a) Achieve more effective coordination of DOE materials research and development;
(b) Assure optimum use of DOE's existing expertise in the field of materials research and development;
(c) Achieve the most rapid communication among the DOE program representatives of new developments, opportunities and problems in the area of materials research and development; and
(d) Provide an infrastructure to facilitate DOE responses to external agency inquiries regarding DOE materials research and development.

The EMaCC shall have the following charter:

I. SCOPE

Materials research and development is defined as research on solids or liquids. Specific topical areas for inclusion or exclusion shall be left to the Committee's judgment. Both applied and basic research are included in the scope. Particular emphasis in the basic research area is placed on those topics interacting with applied efforts although it is recognized that all basic research on materials is not immediately relevant to the applied programs. In the applied programs, emphasis is placed on materials development and materials engineering. It is recognized that this may include economic or scale-up materials problem areas in energy systems. Raw materials and gaseous materials are not to be emphasized by the EMaCC in order to more effectively focus the Committee's objectives.

II. RESPONSIBILITIES

A. Exchange of program, budgetary and planning information: The EMaCC members shall keep their respective divisions or offices informed of pertinent information concerning other division programs.

B. Technical information exchange: Members of the Committee shall provide and receive information to keep informed of the state of materials research and technology.

C. Evaluations: The EMaCC shall identify areas of increased emphasis or areas of opportunity as the need arises; or respond to requests of the Secretary, Assistant Secretaries or the Director of the Office of Science. The EMaCC Chair shall report annually to the Director of the Office of Science with an administrative report and shall provide a copy of this report to the Executive Secretary for retention in the EMaCC file.

D. Reporting: The EMaCC shall keep minutes of each meeting and shall circulate them to all interested DOE personnel. The EMaCC or its members shall report on its activities as the need arises to Office or Division Directors. When appropriate, the Committee may bring certain matters to the attention of the Director of the Office of Science.

E. Annual Technical Report: The EMaCC annually shall publish and distribute an Annual Technical Report summarizing all DOE materials research and development programs.

F. File storage shall be provided by the Division of Materials Sciences and Engineering in the Office of Science. Web hosting will also be provided with the expectation that all involved parties will establish appropriate links.

III. MEMBERSHIP

The EMaCC shall include members from any DOE organizational unit having a substantial interest in materials. An organizational office is defined as any division or office having programmatic responsibilities. Representatives from other federal agencies and from the DOE laboratories may be invited to attend as needed or when appropriate. Employees of DOE laboratories and employees of other organizations with which DOE has contracts may participate as members of EMaCC, except on funding issues which are "not for public release," when assigned to participate in EMaCC while on detail to DOE headquarters in Washington, DC and Germantown, MD. Membership in EMaCC shall be at the discretion of Division/Office Directors.

Any member of EMaCC in attendance at EMaCC meeting is deemed a voting member with regard to any business considered at an EMaCC meeting except for those items specifically reserved to Voting Representatives of the member divisions/offices participating in EMaCC.

The Directors of each Division/Office participating in EMaCC shall designate a member of the staff of that Division/Office to serve as a Voting Representative for EMaCC. Each participating Division/Office shall have one vote. The Voting Representatives will be responsible for electing the Chair and Executive Secretary, for approving all revisions of the Charter and for voting on any other matters that the members of EMaCC may refer to them.

IV. OFFICERS

The EMaCC shall have a Chair and an Executive Secretary to carry out the administrative functions of the Committee. The Chair shall be a Voting Representative. The Executive Secretary need not be a Voting Representative of EMaCC. The Chair and Executive Secretary shall serve for a term of one year and shall be nominated by committee of EMaCC approved at a duly convened EMaCC meeting. The Chair and Executive Secretary shall be elected by the Voting Representatives during the fourth quarter of the fiscal year to serve for the next fiscal year. A quorum of ten Voting Representatives, with at least four of the Voting Representatives from divisions in different assistant secretarial offices, shall be required to elect the Chair and Executive Secretary.

The duties of the Chair shall include:

A. Convening and leading EMaCC meetings

B. Representing the EMaCC as appropriate and involving other EMaCC members in reporting to DOE management and

C. Assuring that the EMaCC abides by this Charter

The duties of the Executive Secretary shall include:

A. Serving in the absence of the Chair

B. Publishing and distributing the meeting notices and minutes

C. Retaining the EMaCC files

D. Publishing the EMaCC Annual Technical Report

V. TOPICAL SUBCOMMITTEES

Topical Subcommittees are responsible for conducting seminars and otherwise facilitating information flow between DOE organizational units with interests in the Subcommittees' respective materials subjects. The functions of the Subcommittees are:

(a) Coordination of efforts in key DOE materials areas
(b) Participation in appropriate interagency meetings in areas of interest
(c) Recommendation of issues and actions to entire EMaCC as appropriate
(d) Provision of input to EMaCC Annual Technical Report

A new Topical Subcommittee can be created at the initiative of any member of EMaCC and with the approval of a duly constituted meeting of EMaCC.

Topical Subcommittee Chairmen shall be appointed by the Chair. The Topical Subcommittee Chairmen shall serve as an advisory committee for the purposes of program planning and preparation of the Annual Technical Report. Each Topical Subcommittee Chair shall prepare an brief annual administrative report to the EMaCC Chair with a copy to the Executive Secretary.

VI. **MEETINGS**

The EMaCC shall determine the frequency with which to hold meetings, provided that Committee shall meet at least three times a year. The Committee shall determine the time, place, and agenda for the next meeting.

VII. **EMaCC ANNUAL REPORT**

EMaCC shall published an Annual Report providing budgetary, programmatic and project information about the various non-classified materials-related programs in DOE. In addition, the Annual Report shall contain brief reports on the activities of EMaCC and other DOE materials activities which EMaCC may deem appropriate to include in the report.

During the months of August or September, the Executive Secretary shall request the submission of budgetary, programmatic and project information pertaining to materials activities of the divisions participating in EMaCC. Divisions will be requested to provide such information by the November 1 in order to assure timely preparation and publication of the Annual Report.

The Executive Secretary shall be responsible for maintaining a current distribution list for the Annual Report.

VIII. **REVISIONS AND AMENDMENTS**

Revisions or amendments of the charter may be proposed by any member of EMaCC for consideration at duly convened meeting. Copies of the proposed revisions or amendments most be provided to the members of EMaCC at least thirty days prior to the meeting in which they will be considered. Upon consideration and approval by two-thirds of those present at an EMaCC meeting, the proposed revisions or amendments shall be presented to the Voting Representatives for approval. Upon approval by two-thirds of the Voting Representatives responding in an EMaCC election, the revisions or amendments shall be accepted.

INDEX

A

B

C

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

Z