DOE/SC-0094

ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 2004

August 31, 2005

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

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INTRODUCTION

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

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

Membership in the EMaCC is open to any Department organizational unit; participants are appointed by Division or Office Directors. The current active membership is listed on pages 4-6.

Five meetings were scheduled for 2004-2005. The dates and minutes from the meetings are as follows:

JULY 20, 2004 - GERMANTOWN

The EMaCC meeting was held in room E-301 Germantown building on Tuesday, July 20, 2004. The meeting started at 10:15 A.M. and ended at 11:40 A.M. The chairman, Dr. Lane Wilson, opened the meeting with participants introducing themselves.

Raul Miranda (BES/SC) talked about Materials Challenges in Catalysts. The talk covered from the basics about catalysis, the nanoscale phenomena, to research examples including design, synthesis and characterization of nanocrystalline catalysts. Future perspectives in the catalysis research were also discussed.

David Berry (NETL/FE) talked about Materials Issues Related to Fuel Reforming Catalysts, including the Solid State Energy Conversion Alliance (SECA) fuel cell program vision: a single mass-manufactured core module. The presentation covered the technical issues and challenges in fuel processing and NETL fuel processing R&D activities.

The minutes of the meeting held on April 22, 2004, were approved.

LIST OF PARTICIPANTS

Doug Archer	FE-24	Douglas.Archer@hq.doe.gov
Dave Berry	FE/NETL	david.berry@netl.doe.gov
Roxanne Danz	EE-2H	Roxanne.Danz@ee.doe.gov
Bob Gottschall	SC-13	Robert.Gottschall@science.doe.gov
Tom Kiess	RW-40E	Thomas.Kiess@RW.DOE.gov
Dale Koelling	SC-13	Dale.Koelling@Science.DOE.gov
Raul Miranda	SC-14	Raul.Miranda@science.doe.gov
Gene Nardella	SC-55	gene.nardella@science.doe.gov
Lane Wilson	FE/NETL	lane.wilson@netl.doe.gov
Mike Soboroff	EA-1	Mike.Soboroff@hq.doe.gov
Jane Zhu	SC-13	jane.zhu@science.doe.gov

FEBRUARY 8, 2005 - FORRESTAL

The EMaCC meeting was held in room 2E069 Forrestal building on Tuesday, February 8, 2005. The meeting started at 10:15 A.M. and ended at 11:40 A.M. The chair, Dr. Lane Wilson, opened the meeting with participants introducing themselves.

Roxanne Garland (EE-2H) gave an overview on Direct Photoelectrochemical Production of Hydrogen. The topics covered includes hydrogen production from visible light and water, photoelectrochemical-based direct conversion systems, photoelectrochemical (PEC) hydrogen production barriers, technical challenges (efficiency, material durability, and energetics), PEC targets, current projects and recent new awards.

David Hamilton (EE-2G) spoke about our need for low cost transportation, more electricity, new power plants and storage, and the concern on the fight for oil resources. Battery technology is improving; the Toyota Prius-II NiMH technology has 50% better performance in all areas than its predecessor. David talked about his interest in recyclable radio nuclide batteries with low or no gamma emission and posed the question: “Are we loosing nuclear technology too?”

The minutes of the meeting held on July 20, 2004, were approved.

Election of 2005 EMaCC new officers are as follows:

Jane Zhu, Chair
Sue Lesica, Executive Secretary

Richard Silberglitt was on travel and couldn’t attend the meeting, but asked Jane to remind people to submit and update the program information for this year’s report (on FY 2004).

The next EMaCC meeting is May 4, 2005, at Germantown, 10:15-11:30 A.M.

Additional calendar items:

a) BES Workshop on Basic Research Needs for Effective Solar Energy Utilization, Bethesda North Marriott Hotel and Conference Center, April 18-21, 2005

b) DOE Hydrogen Program Review, Arlington, VA, May 23-26, 2005 (DOE Coordinator - Carole Read).

c) Basic Energy Sciences Advisory Committee meeting, Omni Shoreham Hotel, Washington, DC, June 6-7, 2005 (contact: Karen Talamini)

LIST OF PARTICIPANTS

Doug Archer	FE-24	Douglas.Archer@hq.doe.gov
Sara Dillich	EE-2F	sara.dillich@ee.doe.gov
Randy Ellingson	SC-13	randy.ellingson@science.doe.gov
Roxanne Garland	EE-2H	roxanne.garland@ee.doe.gov
David B. Hamilton	EE-2G	david.hamilton@ee.doe.gov
Alan Hartman	ARC	hartman@alrc.doe.gov
Sue Lesica	NE-20	sue.lesica@nuclear.energy.gov
Dale Koelling	SC-13	Dale.Koelling@Science.DOE.gov
Raul Miranda	SC-14	Raul.Miranda@science.doe.gov
Lane Wilson	FE/NETL	lane.wilson@netl.doe.gov
Carole Read	EE-2H	carole.read@ee.doe.gov
Mike Soboroff	EA-1	Mike.Soboroff@hq.doe.gov
Charles Sorrell	EE-2F	charles.sorrell@ee.doe.gov
Jane Zhu	SC-13	jane.zhu@science.doe.gov

MAY 4, 2005 - GERMANTOWN - Minutes will be published upon approval

JUNE 28, 2005 - GERMANTOWN - Minutes will be published upon approval

SEPTEMBER 7, 2005 - FORRESTAL - Minutes will be published upon approval

The EMaCC reports to the Director of the Office of Science in his or her capacity as overseer of the technical programs of the Department. This annual technical report is mandated by the EMaCC Charter. This report summarizes EMaCC activities for FY 2004 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 2004 was Dr. Lane Wilson. The compilation of this report was performed by Dr. Susan Lesica, EMaCC Executive Secretary for FY 2005, with the assistance of the RAND Corporation. Financial support was provided by the Materials Subprogram of the Industrial Technologies Program and by the Office of Basic Energy Sciences.

Dr. Jane Zhu
Office of Basic Energy Sciences
EMaCC Chair, FY 2005

TABLE 1
ENERGY MATERIALS COORDINATING COMMITTEE MEMBERSHIP LIST

ORGANIZATION	REPRESENTATIVE	PHONE NO.
ENERGY EFFICIENCY AND RENEWABLE ENERGY		
Building Technologies	Marc LaFrance, EE-2J	202-586-9142
FreedomCAR & Vehicle Technologies		
Automotive Lightweight Vehicle Materials	Joseph Carpenter, EE-2G	202-586-1022
Heavy Vehicle Materials Technologies	James Eberhardt, EE-2G	202-586-9837
Geothermal Technologies		
Geothermal Materials	Raymond LaSala, EE-2C	202-586-4198
Hydrogen, Fuel Cells & Infrastructure Technologies		
Fuel Cell Materials	Carole J. Read, EE-2H	202-586-3152
	JoAnn Milliken, EE-2H	202-586-2480
Industrial Technologies		
Materials Subprogram	Sara Dillich, EE-2F	202-586-7925
Solar Energy Technology		
National Photovoltaic Program	Richard King, EE-2A	202-586-1693
	Ray Sutula, EE-2A	202-586-8064
ELECTRIC TRANSMISSION AND DISTRIBUTION		
High Temperature Superconductivity	James Daley, OE-10	202-586-1165

ORGANIZATION	REPRESENTATIVE	PHONE NO.
SCIENCE		
Basic Energy Sciences		
Materials Sciences and Engineering	Harriet Kung, SC-22.2	301-903-0497
Materials and Engineering Physics	Robert J. Gottschall, SC-22.2	301-903-3978
	Yok Chen, SC-22.2	301-903-4174
	Tim Fitzsimmons, SC-22.2	301-903-9830
	Jane Zhu, SC-22.2	301-903-3811
	W. Oosterhuis, SC-22.2	301-903-4173
Condensed Matter Physics and Materials Chemistry	Richard Kelly, SC-22.2	301-903-6051
	Helen Kerch, SC-22.2	301-903-2346
	Arivinda M. Kini, SC-22.2	301-903-3565
	Dale Koelling, SC-22.2	301-903-2187
	Matesh (Mat) Varma, SC-22.2	301-903-3209
	Jim Horwitz, SC-22.2	301-903-4894
Chemical Sciences, Geosciences and Biosciences	Nick Woodward, SC-22.1	301-903-4061
Fusion Energy Sciences		
Facilities and Enabling Technologies	Gene Nardella, SC-24.2	301-903-4956
Biological and Environmental Research		
Medical Sciences	Roland Hirsch, SC-23.2	301-903-9009
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
NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY		
Advanced Nuclear Research	Susan Lesica, NE-20	301-903-8755
Nuclear Facilities Management	John Warren, NE-40	301-903-6491
	Bob Lange, NE-40	301-903-2915
Space and Defense Power Systems	John Dowicki, NE-50	301-903-7729

ORGANIZATION	REPRESENTATIVE	PHONE NO.
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		
Science and Technology and International	Robert Finch, RW-1	202-586-8886
FOSSIL ENERGY		
Advanced Research	Fred M. Glaser, FE-25	301-903-2786

ORGANIZATION OF THE REPORT

The FY 2004 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 2004 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 2004 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 2004 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 2004
BUILDING TECHNOLOGIES PROGRAM	$2,892,000
FREEDOMCAR & VEHICLE TECHNOLOGIES PROGRAM	$39,595,000
Transportation Materials Program	38,535,000
Automotive Propulsion Materials	2,220,000
Automotive Lightweight Materials	16,650,000
Heavy Vehicle Propulsion Materials	4,725,000
High Strength Weight Reduction Materials	8,840,000
High Temperature Materials Laboratory	6,100,000
Electric Vehicle R&D Program	1,060,000
Advanced Battery Development	1,060,000
GEOTHERMAL TECHNOLOGIES PROGRAM	$310,000
Geothermal Materials	310,000
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM	$10,173,646
Hydrogen Storage Materials Program	7,772,146
Hydrogen Production Materials Program	1,409,000
Fuel Cell Materials Program	992,500
INDUSTRIAL TECHNOLOGIES PROGRAM	$16,051,426
Aluminum Subprogram	5,351,635
Metal Casting Subprogram	643,466
Steel Subprogram	NA[1]
Materials Subprogram	10,056,325
SOLAR ENERGY TECHNOLOGY PROGRAM	$25,156,000
Office of Solar Energy Technologies	25,156,000
National Photovoltaics Program	25,156,000
OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION	$33,650,000
High Temperature Superconductivity for Electric Systems	33,650,000
OFFICE OF SCIENCE	$689,599,712
Office of Basic Energy Sciences	631,276,000
Division of Materials Sciences and Engineering	235,806,000
Division of Scientific User Facilities	395,470,000
Office of Advanced Scientific Computing Research	48,034,712
Technology Research Division	48,034,712
Laboratory Technology Research Program	610,100
Small Business Innovation Research Program	43,926,813
Small Business Technology Transfer Research Program	3,497,799
Office of Fusion Energy Sciences	9,000,000
Office of Biological & Environmental Research	1,289,000

[1]For every project within the American Iron and Steel Institute's (AISI) Technology Roadmap Program (TRP), the funding shown is the budgeted total over the life of the project. Total DOE/ITP TRP funding to date (up to FY05) is $20,541,238. Separate FY04 funding data are not available.

FY 2004 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES (continued)

	FY 2004
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	13,130,000
Office of Space and Defense Power Systems	8,666,000
Space and National Security Programs	8,666,000
Office of Advanced Nuclear Research	4,464,000
Advanced Fuel Cycle Initiative	2,464,000
Nuclear Hydrogen Initiative	2,000,000
NATIONAL NUCLEAR SECURITY ADMINISTRATION	$119,168,000
Office of Naval Reactors	75,800,000
Office of Defense Programs	43,368,000
The Weapons Research, Development and Test Program	43,368,000
Sandia National Laboratories	31,935,000
Lawrence Livermore National Laboratory	11,433,000
OFFICE OF FOSSIL ENERGY	$12,540,000
Office of Advanced Research	12,540,000
Advanced Research Materials Program	6,990,000
Advanced Metallurgical Processes Program	5,550,000
TOTAL	$962,265,784

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	$1,200,000	$1,692,000	$0	$0	$2,892,000
FreedomCAR & Vehicle Technologies Program	$25,165,000	$9,820,000	$2,805,000	$1,805,000	$39,595,000
Geothermal Technologies Program	$310,000	$0	$0	$0	$310,000
Hydrogen, Fuel Cells and Infrastructure Technologies Program	$5,417,500	$3,176,971	$1,279,175	$300,000	$10,173,646
Industrial Technologies Program	$7,554,214	$5,381,732	$3,115,480	$0	$16,051,426
Solar Energy Technology Program	$25,156,000	$0	$0	$0	$25,156,000
Office of Electric Transmission and Distribution	$18,250,000	$12,900,000	$1,500,000	$1,000,000	$33,650,000
Office of Science	$440,802,884	$47,424,612	$201,372,216	$0	$689,599,712
Office of Nuclear Energy, Science and Technology	$11,130,000	$0	$2,000,000	$0	$13,130,000
National Nuclear Security Administration	$119,168,000	$0	$0	$0	$119,168,000[1]
Office of Fossil Energy	$5,515,000	$5,830,000	$795,000	$400,000	$12,540,000
TOTALS	**$659,668,598**	**$86,225,315**	**$212,866,871**	**$3,505,000**	**$962,265,784**

[1]This excludes $61.1 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

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

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

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

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

1. Biomass Program
2. Building Technologies Program
3. Distributed Energy Program
4. Federal Energy Management Program
5. FreedomCAR & Vehicle Technologies Program
6. Geothermal Technologies Program
7. Hydrogen, Fuel Cells & Infrastructure Technologies Program
8. Industrial Technologies Program
9. Solar Energy Technology Program
10. Weatherization & Intergovernmental Program
11. 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, composites, coatings, nanoscale materials, advanced forming, welding and joining, corrosion, erosion, wear and other areas.

BUILDING TECHNOLOGIES PROGRAM

	FY 2004
BUILDING TECHNOLOGIES PROGRAM - GRAND TOTAL	$2,892,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$500,000
Hygrothermal Material Property Measurements & Modeling Upgrades and Applications	500,000
FENESTRATION MATERIALS DEVELOPMENT	$2,392,000
Development of Electrochromic Materials and Coatings	1,999,000
Development of Aerogel Materials for R10/ inch Transparent Window Insulation	393,000

BUILDING TECHNOLOGIES PROGRAM

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

Program objectives are as follows:

1. Develop Advanced Windows that have highly insulating properties, that offer dynamic solar heat gain control, and that 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 Building Codes and Standards;

The DOE contact is Marc LaFrance, 202-586-9142

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

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

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

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

FENESTRATION MATERIALS DEVELOPMENT

2. 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 $501,000, Sage $150,000
SAGE Electrochromic Inc.: Neil Sbar, 507-331-4904

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 initial production phase for skylights, although material enhancements and yield improvements continue to be investigated. Sage is constructing a larger factory that will be capable of producing larger products. Sage won a R&D 100 Award in 2004.

$450,000
LBNL: Steve Selkowitz, 510-486-5064

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

Current tasks are to develop and further characterize the class of variable reflectance electrochromic coatings. Explore alternative metals and replacement of hydrogen-based devices with lithium based electrochemistry. Issues that need to be addressed are morphological changes during cycling, alloying for stability and improved reflectivity, electrolyte interactions, and intralayer conductivity. Specific efforts include: Characterization of spectral optical properties across the complete dynamic switching range; continued investigation of degradation mechanisms in metal hydride systems and development of mitigation strategies; and development of prototype devices using both solid state and gasochromic structures in collaboration with industrial partners. LBNL won a R&D 100 Award in 2004.

$250,000
LANL: Anthony Burrell, 505-667-9342

LANL has demonstrated that ionic liquids are effective components in electrochromic technologies. Chemical and material analyses will be conducted to establish an ionic liquid with dyes that are stable in the presence of Ultra Violet light. Similar electrochromic devices have been commercialized for rear view mirrors, but these are highly unstable in the presence of UV, which is not acceptable 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. 2004 activity has successfully achieved stable UV performance and polymer formation that will withstand the hydrostatic pressure.

DOE $798,000, Rockwell $200,000
Rockwell Scientific Co. Morgan Tench, 805-373-4509

This project addresses the key remaining technical requirements for commercialization of reversible electrochemical mirror (REM) smart window devices. These requirements are uniform switching over large areas, an effective seal for preventing intrusion of oxygen and water, and a suitable counter electrode that can be inexpensively produced over large areas. The uniform switching requirement shall be addressed by developing a gellation method that significantly increases the resistance of the electrolyte, and by using programmed voltage switching that takes advantage of the decrease in mirror electrode sheet resistance resulting from silver mirror formation. The counter-electrode requirement shall be addressed by developing a dot matrix electrode that does not require the expensive photolithography used to fabricate metallic grid counter electrodes. A large-area (30 cm square) demonstration devices shall be built and characterized in terms of optical parameters (visible light transmission, reflectance and haze), mirror uniformity as a function of switching speed, and cycle life.

Keywords: Electrochromic, Dynamic Windows, Solar Heat Gain Coefficient, Solar Control, Ionic Fluids, Reflective Hydrides, Reversible Electrochemical Mirror

3. DEVELOPMENT OF AEROGEL MATERIALS FOR R10/ INCH TRANSPARENT WINDOW INSULATION
   DOE $393,000, Aspen Aerogels $76,000
   DOE Contact: Marc LaFrance, 202-586-9142
   Aspen Aerogels, Inc. Contact: Dan Bullock, (508-691-1172

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

Keywords: Aerogels, Advanced Insulation

FREEDOMCAR & VEHICLE TECHNOLOGIES

	FY 2004
FREEDOMCAR & VEHICLE TECHNOLOGIES - GRAND TOTAL	$39,595,000
TRANSPORTATION MATERIALS PROGRAM	$38,535,000
AUTOMOTIVE PROPULSION MATERIALS	$2,220,000
Technical Project Management	150,000
Low-Cost, High Energy Product Permanent Magnets	300,000
Characterization of Rare Earth Permanent Magnets for Automotive Applications	100,000
Graphite Foam Thermal Management Materials for Electronic Packaging	300,000
Mechanical Characterization of Electronic Materials and Electronic Devices	100,000
Round Pleated Ceramic Fiber Diesel Particulate Filter Cartridge	250,000
Fabrication Of Small Injector Orifices	250,000
Electrochemical NO_x Sensor for Monitoring Diesel Emissions	370,000
Proton Exchange Membrane Materials for Fuel Cell Applications at Elevated Temperature	400,000
AUTOMOTIVE LIGHTWEIGHT VEHICLE MATERIALS	$16,650,000
Automotive Aluminum Research and Development	975,000
Advanced Materials and Process Development	3,150,000
Polymer Composites Research and Development	2,370,000
Low-Cost Carbon Fiber	1,500,000
Recycling	2,000,000
Enabling Technologies	4,170,000
High Strength Steels	2,485,000
HEAVY VEHICLE PROPULSION MATERIALS	$4,725,000
Manufacturing Technology for Cermet Components	0
High-Toughness Materials	100,000
Materials for Exhaust Aftertreatment	300,000
Catalyst Characterization	200,000
Development of NO_x Sensors for Heavy Vehicle Applications	200,000
Electron Microscopy for Characterization of Catalyst Microstructures and Deactivation Mechanisms	200,000
Microstructural Changes in NO_x Trap Materials Under Lean and Rich Conditions at High Temperatures	100,000
Aftertreatment Catalysts Materials Research	0
Catalysts via First Principles	365,000
Durability of Particulate Filters (CRADA with Cummins, Inc.)	300,000
Advanced Materials for Lightweight Valve Train Components	100,000
Engineered Surfaces for Diesel Engine Components	40,000
Cermet Materials for Diesel Engine Wear Applications	100,000
Mechanical Characterization	75,000
NDE of Diesel Engine Components	200,000
Durability of Diesel Engine Component Materials	200,000
Life Prediction of Diesel Engine Components	100,000
Low-Cost Manufacturing of Precision Diesel Engine Components	165,000
Advanced Machining and Sensor Concept	100,000
Advanced Cast Austenitic Stainless Steels for High-Temperature Exhaust Components	160,000
TiAl Nanolaminate Composites	75,000
Synthesis of Powders for Titanium Carbide/Nickel Aluminide Cermets	0
Laser Surface Texturing of Lubricated Ceramic Parts	50,000

FREEDOMCAR & VEHICLE TECHNOLOGIES (continued)

	FY 2004
TRANSPORTATION MATERIALS PROGRAM (continued)	
HEAVY VEHICLE PROPULSION MATERIALS (continued)	
Low Cost Titanium Feedstock Consolidation Process	90,000
High Density Infrared Surface Treatment of Materials for Heavy-Duty Vehicles	70,000
High Temperature Aluminum Alloys	50,000
Titanium Alloys for Heavy- Duty Vehicles	100,000
Mechanical Behavior of Ceramic Materials for Heavy Duty Diesel Engines	300,000
Powder Processing of Nanostructured Alloys Produced by Machining	75,000
Deformation Processes for the Next Generation Ceramics	100,000
High Speed Machining of Titanium	75,000
Walker Process for Stress Relief	40,000
Synthesis of Nanocrystalline Ceramics	45,000
Development of Titanium Components for a Heavy-Duty Diesel Engine Turbocharger	0
Surface Modification of Engineering Materials for Heavy Vehicle Applications	200,000
IEA Implementing Agreement for a Programme of Research and Development on Advanced Materials for Transportation Applications	200,000
Testing Standards	75,000
IEA - Rolling Contact Fatigue	175,000
HIGH STRENGTH WEIGHT REDUCTION MATERIALS	$8,840,000
Application of Innovative Materials	695,000
Lightweight Vehicle Structures	2,765,000
Materials Processing Development	1,775,000
Materials Development	855,000
Enabling Technologies	2,750,000
HIGH TEMPERATURE MATERIALS LABORATORY	$6,100,000
High Temperature Materials Laboratory User Program	6,100,000
ELECTRIC VEHICLE R&D PROGRAM	$1,060,000
ADVANCED BATTERY DEVELOPMENT	$1,060,000
New High-Capacity Electrodes for Lithium-Ion Batteries	250,000
New Polymer Structures for Improved Li Ion Electrolytes	250,000
First-Principles Calculations of Improved Li-Ion Cathode Materials	220,000
Synthesis and Characterization of Cathode Materials for Rechargeable Lithium-Ion Batteries	340,000

FREEDOMCAR AND 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 R&D is conducted to address critical needs of automobiles and heavy vehicles. Another important aspect of these activities is the partnership between the Federal Government Laboratories and U.S. industry, which ensures that the R&D is relevant and that federal research dollars are highly leveraged.

Within OFCVT, the bulk of the materials R&D is carried out through Materials Technologies, with additional specialty materials R&D in Electric Drive Vehicle Technologies.

The Propulsion Materials Technologies Development Area develops: (a) *Automotive Propulsion Materials* to enable advanced propulsion systems for hybrid vehicles, and (b) *Heavy Vehicle Propulsion System Materials.* In collaboration with U.S. industry and universities, efforts in heavy vehicle propulsion system materials focus on the materials technology critical to the development of the low emission, 55 percent efficient (LE-55) heavy-duty and multi-purpose Diesel engines, such as: manufacturing of ceramic and metal components for high-efficiency turbocharger and supercharger; thermal insulation, for reducing engine block cooling, lowering ring-liner friction and reducing wear; high-pressure fuel injection materials; and exhaust after treatment catalysts and particulate traps. The DOE contacts are Rogelio Sullivan, 202-586-8042, for Automotive Propulsion Materials and James Eberhardt, 202-586-9837, for Heavy Vehicle Propulsion Materials.

Lightweight Materials Technology Development focuses on two areas: (a) *Automotive Lightweighting Materials (ALM)* and (b) *High Strength Weight Reduction Materials (HSWR)* to reduce vehicle weight and thereby decrease fuel consumption. Automotive Lightweighting Materials seeks to develop advanced materials with the required properties and the processes needed to produce them at the costs and volumes needed by the automotive industries. Improved materials for body, chassis, and powertrain are critical to attaining the challenging performance standards for advanced automotive vehicles. In the area of High Strength Weight Reduction Materials, energy savings from commercial trucking is possible with high strength materials which can reduce the vehicle weight within the existing envelope so as to increase payload capacity, thereby reducing the number of trucks needed on the highways. Increased safety can be obtained by new brake materials and by incorporating highly shock absorbent materials in truck structures for improved control and crashworthiness. The DOE contacts are Joseph Carpenter, 202-586-1022, for Automotive Lightweighting Materials and James Eberhardt, 202-586-9837, for High Strength Weight Reduction Materials.

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

The Electric Vehicle R&D program includes the support of Advanced Battery Development for electric and hybrid vehicle applications. The DOE contact is Ray Sutula, 202-586-8064. Two different programs fund research into new battery materials and battery additives. Advanced Technology Development (ATD) addresses barriers specific to lithium ion technology for high-power applications by focusing on understanding and addressing factors that control key barriers: abuse tolerance, cost, calendar life, and low-temperature performance. The program involves the expertise of five national laboratories (ANL, BNL, INL, LBNL, and SNL), the Army Research Laboratory, industry, and universities (IIT, Illinois, Berkeley, and Wisconsin). Batteries for Advanced Transportation Technologies (BATT) conducts innovative, cutting-edge research on the next generation of lithium battery systems, specifically investigating advanced materials that promise greatly increased power and energy and developing advanced diagnostic tools to investigate failure mechanisms. This program involves three national laboratories (ANL, BNL, and LBNL), industry, and several universities (Berkeley, BYU, Clemson, MIT, Michigan State, SUNY, Michigan, NC State, Texas, and Utah).

TRANSPORTATION MATERIALS PROGRAM

AUTOMOTIVE PROPULSION MATERIALS

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

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

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

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

The objective of this work is to develop a low-cost process for the fabrication of high strength NdFeB permanent magnets (PMs) to enable significant size and weight reductions of traction motors for hybrid electric vehicles. A facility was established at Argonne National Laboratory for pressing permanent magnets in the high fields (9 T) of a superconducting solenoid. In FY 2004, we modified the hydraulic loop for better indication and control of the pressure during initial stage of the compact pressing operation. A new glove box, for better control of oxygen during pre- and post-compact-press operation, was procured and installed. The new glove box can provide an oxygen environment of less than 300 parts per million, which is needed in order to avoid oxidation of the powder and degradation of the magnetic properties of the permanent magnet. We fabricated, with limited success, a number of near-final-shape compacts with L/D ratio smaller than 0.25 in various alignment fields from 1 to 8 T. These compacts are quite fragile because they are very thin (only 3.3 mm thick) and must be handled with extreme care. The success rate is rather low (~25 percent). We still do not know exactly what causes the compact to fail (crack) after ejection from the die although we suspect the main culprit is trapped air. We need to improve the success rate in the future. We completed a conceptual design of a semi-automated superconducting PM fabrication system, which includes mainly a dual-ended, four-position, horizontal press system and an actively shielded, helium-cooled, superconducting magnet with a horizontal room-temperature bore. The horizontal press can be slid in and out of the bore of the superconducting magnet. The four arms of the press, 90 degrees apart, rotate around a pivot point. The four positions represent the pressing, ejection, cleaning, and filling stations. We contracted Data Decisions to conduct an economic study of the superconducting PM manufacturing system. The main objective is to compare the cost of manufacturing PMs using the superconducting technology and conventional technology using electromagnets. A preliminary report of the economic study was issued during FY 2004.

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

6. CHARACTERIZATION OF RARE EARTH PERMANENT MAGNETS FOR AUTOMOTIVE APPLICATIONS
   $100,000
   DOE Contact: R. Sullivan, 202-586-8042
   ORNL Contact: D. P. Stinton, 865-574-4556
   ORNL Principal Investigator: Edgar Lara-Curzio, 865-574-1749

The development of higher energy permanent magnets for drive motors of electric vehicles offers an opportunity for significant weight reduction. At ORNL, work has been carried out to characterize sintered and bonded permanent magnets fabricated under different conditions. The magnetic properties are impacted by the grain size, the texture (or preferred orientation), and the impurity phases. Crystallite size, texture, and composition are all features that can be determined using X-ray diffraction and electron microscopy.

Before their widespread use in electric vehicles, it is critical to determine the effect of the operating environment on the magnetic and mechanical properties of candidate bonded and sintered permanent magnets. For example, these materials should be capable of retaining their magnetic and mechanical properties after repeated thermal cycling. To this end, ORNL studied the evolution of the magnetic and mechanical properties of sintered and bonded permanent magnets as a function of thermal cycling between –40˚C and 150˚C. This was accomplished by using a specially designed environmental chamber that allows the in-situ evaluation of the magnetic strength of the materials evaluated as a function of temperature and number of thermal cycles. This work was carried out in Collaboration with magnet suppliers.

ORNL also continued providing texture characterization of magnets synthesized at ANL . Additional microstructural characterization included information on chemical composition, crystallite size, and the preferred orientation to further refine the alignment process.

Additionally, characterization support was provided for extruded isotropic magnets and magnetic powders produced by the OAAT-funded project led by Dr. Anderson at Ames Laboratory.

Keywords: NdFeB, Permanent Magnets

7. GRAPHITE FOAM THERMAL MANAGEMENT MATERIALS FOR ELECTRONIC PACKAGING
   $300,000
   DOE Contact: R. Sullivan, 202-586-8042
   ORNL Contact: D. P. Stinton, 865-574-4556
   ORNL Principal Investigator: Nidia Gallego, 865-574-5220

The goal of this program is to utilize high conductivity graphite foam in heat spreaders, heat sinks, and other components in order to cool or to improve the thermal management of electronics. Previous work has demonstrated that when graphite foam is utilized as the core material for a heat sink, the effective heat transfer can be significantly increased compared to traditional materials and designs. A mathematical model was developed to predict the thermal performance of the foam in heat sink applications. However, the current model needs to be expanded to relate materials parameters (i.e., pore size, window size, density, anisotropy, etc.) to the thermal properties for use in a power electronic thermal management system.

Work will continue to evaluate and optimize Carbon Foam for conventional finned heat sink applications. In addition, work addressing the fundamental understanding of the durability of the foam will be pursued. Vibration, corrosion, debris fouling, thermal cycling, and other relevant properties will continue to be evaluated for the new compositions with optimized pore size, density, etc. In order to capitalize on the modeling effort, the thermal conductivity of carbon foam and the microstructure will be optimized. Work will focus on understanding the different modes of evaporative cooling (pool boiling, spray cooling and thin film evaporation) and the role of the evaporant effect thermal transfer. Partnerships with commercial manufacturers or end users will be necessary in order to correctly address the critical needs for each application. Industrial partners such as Intel, Visteon, Delphi, GM, and 3M will be approached for collaboration.

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

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

A major focus of the Power Electronics effort in the Automotive Propulsion Materials Program is to develop polymer capacitor technology that will replace current electrolytic, dc buss capacitors for power electronic modules in electric hybrid vehicles. The ultimate objective is to make the power modules more compact while still maintaining the tight voltage and temperature requirements and long service life without compromise from mechanical breakdown of the dielectric film. Toward that end, collaboration with Sandia National Laboratory (SNL) exists to mechanically evaluate a suite of SNL-manufactured hydroxylated polystyrene (PVOH) dielectric polymers that have potential to satisfy the above objectives. The present Subtask works toward satisfying two of its own goals: measure baseline mechanical properties of that suite of PVOH compositions and interpret their results so to suggest which are most suitable for manufacturing scale-up, and quantify the mechanical performance those manufactured films so ultimate manufacturers and end-users of these dielectric films may use them without mechanical breakdown.

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

9. ROUND PLEATED CERAMIC FIBER DIESEL PARTICULATE FILTER CARTRIDGE
   $250,000
   DOE Contact: R. Sullivan, 202-586-8042
   ORNL Contact: D. P. Stinton, 865-574-4556
   Industrial Ceramic Solutions Contact: R. Nixdorf, 865-482-7552

In the FY 2003 ICS work, a new product alternative to control diesel particulate across all market applications emerged. This was the round ceramic fiber pleated filter cartridge. All of the approaches to PM control must use some form of a ceramic filter. To date, that filter choice has been an extruded honeycomb “wall-flow” product. Experiments conducted by ICS and others under the FY 2003 program demonstrated much less exhaust backpressure on the diesel engine with the pleated ceramic fiber DPF. This will improve engine performance and reduce the fuel penalty imposed by the PM control device. The pleated ceramic fiber DPF, which weighs significantly less than the extruded wall-flow filter, exhibited a lower thermal mass to achieve faster soot combustion temperatures and adds less weight to the vehicle. Customer performance testing during FY 2004 of the improved round pleated diesel particulate filter proved that the ICS filter is a viable solution to the diesel exhaust emissions 2007 regulations. ICS located a filter manufacturing partner in early FY 2004 who is capable of the large volume quantities required by vehicle OEMs.

Keywords: Carbon Particulates, Diesel, Filters, Microwave Regeneration

10. FABRICATION OF SMALL INJECTOR ORIFICES
    $250,000
    DOE Contact: R. A. Sullivan, 202-586-8042
    ORNL Contact: D. P. Stinton, 865-574-4556
    ANL Contact: G. R. Fenske, 630-252-5190

Decreasing the size of fuel injector orifice holes enhances atomization of fuel in CIDI engines and thus presents a potential approach to achieve more stringent particulate emission standards. Currently, electrodischarge machining can routinely by used to fabricate orifices as small as 100 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. Bench scale tests demonstrated the ability to reduce the diameter of 200 mm diameter norifices down to 50 mm. Efforts were initiated this past year to transfer the process to a commercial coating company. A series of nozzles were successfully coated to produce 80 mm diameter orifices on a commercial nozzle. Efforts are underway to limit the coating to selective areas of the injector to the orifice region only and to prepare nozzles for fuel spray and engine emission studies. Studies were also initiated to investigate the impact of the coatings on deposit formation - a critical issue for small orifices.

Keywords: Fuel Injectors, Nozzles, Orifice, Coating

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

The purpose of the proposed research is to develop technology for low cost, high sensitivity, on-board sensors for the detection of NO_x in diesel exhaust. The sensors will be based upon metal oxide/solid electrolyte technology which has demonstrated significant potential for the detection of hydrocarbon emissions in automobile exhaust. Sensor material and design will be optimized for an environment comparable to the exhaust stream of the CIDI engine. The project is being performed in collaboration with Ford Research and Advanced Engineering and Oak Ridge National Laboratory. Critical path tasks for commercialization of the sensor are being shared by the three organizations (LLNL, ORNL and Ford) based on their expertise and support. Current efforts at LLNL are focused on characterization of aging mechanisms during sensor operation. Changes in surface stoichiometry, electrode microstructure, and electrode/electrolyte interface structure have been observed to occur during aging of the sensors over several weeks. The impact of the observed aging processes on the NO_x sensing characteristics is currently under investigation.

Keywords: NO_x, Electrochemical Sensor, CIDI, Diesel Exhaust

12. PROTON EXCHANGE MEMBRANE MATERIALS FOR FUEL CELL APPLICATIONS AT ELEVATED TEMPERATURE
    $400,000
    DOE Contact: R. A. Sullivan, 202-586-8042
    ORNL Contact: D. P. Stinton, 865-574-4556
    ORNL Principal Investigator: Mike Simonson, 865-574-4986
    University of Southern Mississippi Contact: K. A. Mauritz

Robust, highly conductive, and inexpensive proton exchange materials (PEMs) are needed for practical and reliable fuel cell operation at elevated temperatures. The current class of PEM fuel cells operating at 90˚C is plagued by sensitivities to CO and peroxide formation that limit performance and require the use of high purity fuels. A polymeric membrane able to operate at elevated temperatures ($\geq$120˚C) would eliminate issues with CO since at these temperature CO adsorption is no longer kinetically favorable. The nature of the polymeric membrane plays a crucial role in determining the performance of the fuel cell. Unfortunately, current membranes based on polymers such as Nafion suffer serious disadvantages including high cost (>$800/m^2) and limited thermal stability at temperatures above 100ºC. We will address the clear need for improved PEM materials through a coordinated program of novel material synthesis, characterization, and testing, with ultimate goal the demonstration of capabilities of new classes of PEMs for sustained operation at elevated temperature (120˚C).

Keywords: PEMs, Fuel Cells

AUTOMOTIVE LIGHTWEIGHT MATERIALS

13. AUTOMOTIVE ALUMINUM RESEARCH AND DEVELOPMENT
$975,000
DOE Contact: Joseph Carpenter, 202-586-1022
ORNL Contact: Phil Sklad, 865-574-5069
PNNL Contact: Mark Smith, 509-375-4478
Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory
Industry Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors), Boeing

The objectives of this effort are: to develop electromagnetic forming (EMF) technology that will enable the economic manufacture of automotive components from aluminum sheet; to experimentally validate stress-based forming limits; to validate enhanced formability through the application of non-proportional loading; to develop and demonstrate, on an industrial scale, an optimized, closed-loop, flexible binder control system to improve the quality of stampings made from aluminum alloys; to develop and demonstrate a production process for the warm forming of aluminum for automotive body structures; and to demonstrate concept feasibility of infrared thermal forming of aluminum tubes.

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

14. ADVANCED MATERIALS AND PROCESS DEVELOPMENT
$3,150,000
DOE Contact: Joseph Carpenter, 202-586-1022
ORNL Contact: Phil Sklad, 865-574-5069
Laboratory Partners: Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Sandia National Laboratories
Industry Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors), Visteon, Westmoreland, EKK, American Foundryman's Society, Stackpole Ltd., Valimet, Aluminum Consultant's Group, Eck Industries, Meridian, Spartan Die Casting, Lunt Industries.
University Partners: Georgia Tech University, Mississippi State University, University of Kentucky, University of Tennessee

The objectives of this project are to develop the tools that will be used to enhance the application of lightweight metals in automotive components. Activities include: numerical simulation modeling to predict mold cavity fill and casting solidification for die cast components; simulation models that predict cast component monotonic and cyclic properties; development of non-destructive evaluation equipment, procedures, and process sensors; demonstration of a production-intent process scheme for titanium alloy powder metal components; development of processing technologies for low-cost metal matrix composite (MMC) materials that are cost competitive with typical aluminum alloys used in the automotive industry; demonstration of the feasibility and benefits of using magnesium alloys in place of aluminum in structural powertrain components; and development of lightweight glazing systems.

Keywords: Magnesium, Cast Metals, Automotive, Die Casting, Simulation Modeling, Glazing, Powder Metallurgy, Titanium Alloy Powders, Aluminum Metal Matrix Composites

15. POLYMER COMPOSITES RESEARCH AND DEVELOPMENT
$2,370,000
DOE Contact: Joseph Carpenter, 202-586-1022
ORNL Contact: Phil Sklad, 865-574-5069, Dave Warren, 865-574-9693
Laboratory Partners: ORNL
Industrial Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors)

The objectives of this project are to define and conduct vehicle related R&D in polymer composite materials processing. Activities include: development of technologies to cost effectively process composite materials into automotive components, integration of these technologies into demonstration projects that display cost effective use of composites that can be manufactured in automotive factories, development of advanced vehicle system designs based on composite materials to both define future research needs and demonstrate the technical and economic viability of developing technologies. Individual activities include: Composite Intensive Body Structure Development, High-Volume Processing of Composites, and Development of Manufacturing Methods for Fiber Preforms. A portion of this effort is devoted to developing the next generation programmable processing machine.

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

16. LOW-COST CARBON FIBER
    $1,500,000
    DOE Contact: Joseph Carpenter, 202-586-1022
    ORNL Contact: Dave Warren, 865-574-9693
    Laboratory Partners: Oak Ridge National Laboratory
    University Partners: Clemson University, Virginia Technological University
    Industry Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors)/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

17. RECYCLING
    $2,000,000
    DOE Contact: Joseph Carpenter, 202-586-1022
    ORNL Contact: Phil Sklad, 865-574-5069
    ANL Contact: Ed Daniels, 630-252-5279
    Laboratory Partners: Argonne National Laboratory
    Industry Partners: Vehicle Recycling Partnership (DaimlerChrysler, Ford, General Motors)

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

18. ENABLING TECHNOLOGIES
    $4,170,000
    DOE Contact: Joseph Carpenter, 202-586-1022
    ORNL Contact: Dave Warren, 865-574-9693
    PNNL Contact: Mark Smith, 509-375-4478
    Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory
    Industry Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors), Dow, Goodrich, Baydur Adhesives, Edison Welding Institute
    University Partners: University of Tennessee, University of Tulsa, University of Michigan, University of California-Santa Barbara, University of Cincinnati, Wayne State University, Stanford University, University of Nottingham

The objective of this effort is to develop technologies that remove barriers to implementation of lightweight materials in automotive applications. In particular, activities include: development of non-destructive evaluation and testing techniques that are sufficiently fast, robust in the manufacturing environment, accurate and cost-effective to be suitable for on-line inspection of spot-welded automotive structures; development of joining technologies and evaluation of joint performance for dissimilar aluminum and aluminum-steel materials in automotive applications; development of coupled thermo-electric, mechanical-metallurgical models of electrode deformation during resistance spot welding of galvanized steel and aluminum; development of 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; development of innovative attachment techniques for joining materials subjected to crash scenarios; development of numerical methods and guidelines in order to realistically assess the influence that the properties of strain rate dependent materials exert in crashworthiness computations; development of the capability of testing new lightweight materials at strain rates comparable to those observed in automobile crashes; and development of experimentally-based, durability driven guidelines to assure the long term integrity of carbon-fiber-based polymeric composite automotive structures in various environments. Projects are conducted by multi-organizational teams involving

USAMP members, automotive suppliers, universities, national laboratories and private research institutions.

Keywords: Polymer Composites, Aluminum, Magnesium, Adhesive Bonding, Welding, Spot Welding, Durability, Joining, Dissimilar Materials, NDE, Strain Rate, Crashworthiness, Numerical Modeling

19. HIGH STRENGTH STEELS
    $2,485,000
    DOE Contact: Joseph Carpenter, 202-586-1022
    ORNL Contact: Phil Sklad, 865-574-5069
    PNNL Contact: Mark Smith, 509-375-4478
    Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory
    Industry Partners: American Iron and Steel Institute, Auto/Steel Partnership, Ford, General Motors, DaimlerChrysler, Ispat Inland, US Steel, Roman Engineering, Dofasco, Stelco
    University Partners: Oakland University, University of Toledo, University of Missouri, University of Dayton Research Institute, Westmoreland, Tribsys Inc., Altair Engineering, Magna International

The objective of this effort is to identify technologies necessary to allow the automotive industry to take advantage of the properties of Advanced High Strength Steels (AHSS) in order to reduce weight and improve performance of future automobiles. Barriers exist in the area of forming, joining, and design. Activities include: developing numerical modeling guidelines to assess the influence that properties of strain-rate-dependent materials have on crashworthiness computations; to develop a methodology to facilitate the forming of AHSS; developing accurate prediction and control methods for controlling springback during stamping processes; investigating the fatigue life of welded joints in AHSS; developing experimental and modeling approaches for the characterization of crashworthiness and strain rate sensitivity of AHSS; and investigating the effects of tribological conditions on the stamping performance of AHSS.

Keywords: Strain Rate, Crashworthiness, Numerical Modeling, Stamping, Advanced High Strength Steels (AHSS), Crashworthiness, Springback, Tribology

HEAVY VEHICLE PROPULSION MATERIALS

20. MANUFACTURING TECHNOLOGY FOR CERMET COMPONENTS
    $0
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    SIUC Contact: Dale Wittmer, 618-453-7006

This task will have two major components:

a. Continue to develop low-pressure injection molding and extrusion techniques for intermetallic bonded carbides and cermets.

   During the previous funding cycle, we used our low-pressure injection molder to form several batches of intermetallic bonded TiC. The formed cermets were sintered by both continuous sintering at SIUC and by the V-LPHIP process at ORNL. Several of these formulations were processing into small cylindrical shapes that could be further machined for diesel engine components. These shapes were continuously sintered, machined into test shapes and tested for density, hardness and strength. Although the V-LPHIP process as ORNL produced the highest density and hardest parts, continuous sintering produced parts sufficiently dense and hard to warrant further study. Also continuous sintering has been proven to be a cost effective manufacturing method for other materials. Presently we have designed a mold for a fuel injector prototype and that mold is currently being fabricated. In addition, the effect of high heating rates on densification is being explored.

b. Develop cost modeling for cost effective processing for both pre-alloyed and reaction sintered intermetallic bonded TiC.

   In this task a cost model was developed to compare conventional processing and sintering to the cost effective processing and sintering methods developed in this and previous modifications. Current production methods use vacuum sintering and HIPing as standard methods, while the cost effective method developed at SIUC uses a continuous furnace under flowing inert gas. As part of this comparison, the use of pre-alloyed metal powders was compared with the use of the individual (non-alloyed) metal powders that are used in the reaction sintering method. It appears from preliminary results, that some intermetallic bonded-TiC formulations can be processed with cost similar to those for high purity oxide ceramics. However, the intermetallic has the ability to be much more cost effective because it can be machined by electro-discharge machining (EDM) while the ceramics must be diamond machined.

Additional processing steps, such a sintering cycle time are being explored to refine the present model.

Keywords: Cermets, Intermetallics, Manufacturing Technology

21. HIGH-TOUGHNESS MATERIALS
$100,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832

Significant improvement in the reliability of structural ceramics for advanced diesel engine applications could be attained if the critical fracture toughness (K_{1c}) were increased without strength degradation. At the same time, cost is a major factor in determining the applicability of new materials in engine components. Thus, 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. However, when the economics of producing the TiC-Ni_3Al composites was examined a significant cost was associated with the use of the NiAl precursor powder. In fact, at the present time the NiAl alone constituted about 55 percent of the total raw material cost. Because the costs of the starting raw materials can be a significant fraction of the total cost of a component, alternative materials for fabricating the cermets are of interest. Previous efforts assessed alternate NiAl sources for cost-effective composite production and identified some that have potential to significantly reduce costs. In general, it was found that the alternative precursors densified adequately, but the mechanical properties were not sufficient for engine application. Refinement of the processing parameters with the alternate precursors is needed to improve the mechanical performance and will be done in the year of the project. Alternate NiAl sources to be used for the project include an Al-Ni catalyst material, TiC-Ni_3Al mixtures developed by the University of Colorado, and Ni-Al-TiC blends for reaction synthesis. In addition, the project will continue to work with CoorsTek Inc. (a parts supplier) for scale-up of the processing and to supply them with pilot plant scale quantities of powder mixtures for injection molding trials. Sintered parts produced in conjunction with CoorsTek will be supplied to Cummins, Inc. for rig testing of machined components.

Keywords: Cermets, NiAl, TiC

22. MATERIALS FOR EXHAUST AFTERTREATMENT
$300,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
Caterpillar Contact: Craig Habeger, 309-578-4468

The proposed program will cover the following technologies.

a. Lean-NO_x Catalysis - Because of the inherently low hydrocarbon concentration in diesel exhaust, any NO_x reduction catalyst will require the addition of supplemental reductant to achieve required NO_x reduction performance goals. From a diesel engine user's standpoint, the best reductant to use in conjunction with aftertreatment systems is diesel fuel. Unfortunately, the natural form of diesel fuel does not work well with state-of-the-art lean NO_x catalysts because the fuel contains a large portion of hydrocarbons that are relatively inert for the NO_x reduction process over the catalysts. Therefore, the study will focus on the identification of ideal combinations of catalyst materials and specific reductants that will demonstrate high NO_x reduction among known lean NO_x catalytic aftertreatment systems. The reductants to be evaluated in this study will be selected based on availability and feasibility from blended diesel fuels.

b. NO_x sensor - The objective of this research is to develop NO_x sensing technologies that are capable of measuring accurately to 1-5 ppm NO_x in the diesel exhaust environment. Integrating NO_x control aftertreatment with the engine is extremely important to reduce the fuel penalties associated with many of the control strategies. For most aftertreatment strategies, multiple NO_x sensors will be required to monitor exhaust NO_x levels as an on-board diagnostic tool and to control the aftertreatment device/engine for maximum fuel efficiency. Diesel engine test results of the state-of-the-art sensor materials have demonstrated that durability and response time need to be significantly improved for diesel exhaust applications. The current research will focus on improving durability and response time of current state of the art sensors, in particular, amperometric type sensors. Work will investigate the development of electrodes that are not catalytic for NO_x reduction. Further research will focus on developing alternative technologies for sensing NO_x in the diesel exhaust environment that are based on potentiometric and ultraviolet/visible radiation sensing. Milestone: Evaluate novel NO_x sensor in the presence of complex simulated gas mixture.

c. PM Trap - This project will focus on understanding physical and chemical interactions of soot and catalyzed filter materials during regeneration. Development of deep bed filtration materials and performance comparisons of catalyzed DPFs based on deep bed and surface filtration will be performed. The research will utilize a bench-scale diesel burner, which was developed for this project, for characterization of filters. In addition, the structure/property relationships of materials for deep bed soot filtration will be determined. The deep bed filtration media will include sintered metal, wall flow, sintered metal fibers, and sintered ceramic.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

23. CATALYST CHARACTERIZATION
$200,000
DOE Contact: James Eberhardt, 202-586-9837
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, exhaust aftertreatment may be necessary in diesel engines. Currently, no commercial “off-the-shelf” technologies are available to meet these standards. The technology necessary for 2007 will need to integrate aftertreatment with engine controls. Consequently, Cummins, Inc. is working to understand the basic science necessary to develop these systems 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 an exhaust aftertreatment system with improved final product performance in order to meet the 2007 emission requirements. In the FY03 effort, baseline characterizations continued for new materials from various stages of the catalyst’s lifecycle. The surface adsorbing species during nitration and sulfation were identified via spectroscopy. *Ex-situ* microstructural, microchemical and crystallographic studies of these new materials in simulated engine environments were initiated.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

24. DEVELOPMENT OF NO_x SENSORS FOR HEAVY VEHICLE APPLICATIONS
$200,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832

NO_x sensors are 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. The development of a mixed potential sensor is being pursued. This type of sensor is simpler, will be lower in cost and have a higher output signal than current pumping cell sensors under development. The sensor will operate at 700˚C to enable sensing of NO (i.e., reduction of NO_2 to NO) and will eliminate all influence of hydrocarbons, by incorporation of a hydrocarbon catalyst. During the first year of this project ORNL demonstrated that the oxygen sensitivity all mixed potential sensors have can be completely eliminated through use of novel materials. Further, the team developed and tested numerous sensing electrode materials and found several that produce large signals (>100mV) for NO_2.

This task seeks to develop catalytically selective electrodes that will facilitate the development of simple mixed potential NO_x and ammonia sensors. The research will continue the development of mixed conducting oxide powders as NO_x sensing electrodes; the evaluation of the kinetics at the surfaces of these materials with and without an applied electric potential, explore new electrode configurations that may lead to enhanced sensitivity; and finally, the development of low-cost sensors that can either measure total NO_x or be NO specific based on materials and designs developed.

Keywords: Sensors, NO_x, Exhaust Aftertreatment

25. ELECTRON MICROSCOPY FOR CHARACTERIZATION OF CATALYST MICROSTRUCTURES AND DEACTIVATION MECHANISMS
$200,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832

The development of catalysts for removing NO_x and SO_x emissions (by direct reaction and/or by trapping), and for eliminating carbon-based particulates from diesel engine exhausts is a challenging chemical problem. Although substantial effort has been devoted to understanding and improving such catalysts, there is no known catalyst that meets all the requirements necessary for commercial applications. For example, several catalyst materials have been reported in the open literature to show promising performance for urea or hydrocarbon SCR (selective catalytic reduction) of NO_x. However, little effort has been devoted to systematically investigating the relationship between the surface structure of active metal oxides on support materials, and their catalytic activity. Therefore, the reaction mechanism and the deactivation or poisoning effects of active sites are not yet fully understood. In like fashion, catalysts for trapping NO_x and SO_x emissions and for trapping and burning particulates still must be perfected, and the problems with aging (related to thermal, hydrothermal, sulfation-desulfation effects) need to be overcome. Because the catalytic reactions are controlled largely by the *nature* of catalytic species (chemistry, morphology, support interactions, etc.) at the atomic level, it is increasingly important to understand the ultrastructure of these materials at the atomic level. The advanced sub-Ångström (Å) imaging capabilities offered by ORNL's new aberration-corrected electron microscope (ACEM), a STEM-TEM instrument due to be delivered by JEOL, USA in the spring of 2004, will be exploited to provide the highest resolution imaging and spatial resolution energy-loss spectroscopy in the world. As part of this project, the HTML has a newly operational JEOL field-emission STEM-TEM instrument with 1.6Å imaging in dark-field, which we are incorporating into our program for characterizing catalytic materials at the near-atomic level. The 2010F will be outfitted with a specimen holder compatible with the HTML's ex-situ catalytic reactor, which is currently being modified to allow more controlled studies of catalytic materials. This will allow studies of the nature of catalysts, leading to an understanding of reaction mechanisms and failure modes in a variety of materials of current interest. These include catalyst materials for emission abatement, catalysts for fuel cells, and hydrogen storage materials, for example.

The objective of the proposed research is to investigate the nature of the active sites of promising metal oxide materials [e.g., Pt and Pd on ceria-zirconia materials for reactions in particulate traps to eliminate soot (with NTRC, in conjunction with the CLEERS program, per Stewart Daw) and ceria-zirconia-lanthana mixtures on BaO- Al_2O_3 supports for NO_x trapping applications, with Ford Research Laboratory] so that the catalytic performance can be improved further through a proper design of catalyst preparation processes or an addition of necessary catalytic "promoters." Transmission electron microscopy and "Z-contrast" scanning transmission electron microscopy will be combined with XPS to determine the effect of aging on the surface structure and dispersion of heavy metal species on oxide supports. The analytical capabilities of the JEOL 2010F will primarily be used. This will also contribute to the experience base needed to rapidly realize the full potential of the ACEM when it begins beneficial operation.

Keywords: TEM, Catalyst, Microstructure

26. MICROSTRUCTURAL CHANGES IN NO_X TRAP MATERIALS UNDER LEAN AND RICH CONDITIONS AT HIGH TEMPERATURES
    $100,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

Our recent results of microstructural analyses of fresh and aged supplier NO_x traps (Ford provided) have lead to some very interesting conclusions. In two-layer traps (inner Pt/BaO-Al_2O_3 layer and outer Rh/CeO_2-ZrO_2 layer), upon aging, 1) the platinum group metals (Pt, Rh) migrate and sinter to 40-50 nm particles, 2) some Pr-Rh alloy formation occurs, and (3) barium oxide remains uniformly distributed in inner layer and a portion of it migrates into the outer layer. These results show that the lost Pt-BaO surface area leads to decreased NO_x trap performance upon aging. These aging results are different from the current view of aging that assumes that only NO_x absorbers form aluminates. Thus the thermal stabilization efforts were focused on the search for thermally stable NO_x absorbers-alumina system. The PI, while at Ford, showed that addition of transition metals, which catalyze NO_x oxidation, to the trap formulation can eliminate the formation of aluminates, since aluminates react with transition metal nitrates to form barium nitrates.

As part of this project, in collaboration with Ford, we have completed the study of "fresh" Pt/BaO-6Al_2O_3 model compounds prepared by ball-milling and impregnation methods. The *ex-situ* reactor at ORNL is being updated to enable the control of diesel and gasoline lean and rich (simulated) environments. We anticipate completing the study of microstructural changes under lean conditions in the next quarter, using techniques of electron microscopy, X-ray analysis and surface analysis. We then plan to study the changes under rich and lean-rich conditions. Based on the results, we will synthesize new materials that could sustain trap performance despite exposure to NO_x trap operating conditions, and study microstructural changes in the new materials under lean and rich conditions.

Keywords: NO_x Trap Materials, NO_x Absorber Components

27. AFTERTREATMENT CATALYSTS MATERIALS RESEARCH
    $0
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Cummins Contact: Randy Stafford, 812-377-3279

This effort will address research in two major areas of diesel exhaust aftertreatment:

a. Abatement of diesel soot - This research area is focused on the following 3 issues: developing novel catalytic materials for efficient soot oxidation, the effect of microwave heating on the efficiency of soot generation, and developing advanced techniques for probing the degradation of soot filters. The following tasks will be performed:

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

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

Keywords: Diesel Engine, Exhaust Emissions, Particulate Emissions

28. CATALYSTS VIA FIRST PRINCIPLES
    $365,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

This task presents an integrated approach between computational modeling and experimental development, design and testing of new catalyst materials that we believe will rapidly identify the key physiochemical parameters necessary for improving the catalytic efficiency of these materials.

The typical solid catalyst consists of nanoparticles on porous supports. The development of new catalytic materials is still dominated by trial and error methods, even though the experimental and theoretical bases for their characterization have improved dramatically in recent years. Although it has been successful, the empirical development of catalytic materials is time consuming and expensive and brings no guarantees of success.

Experimental catalysis has not benefited from the recent advances in high performance computing that enable more realistic simulations (empirical and first-principles) of large ensemble of atoms, which includes the local environment of a catalyst site in heterogeneous catalysis. These types of simulations, when combined with incisive microscopic and spectroscopic characterization of catalysts, can lead to a much deeper understanding of the reaction chemistry that is difficult to decipher from experimental work alone.

Thus, a protocol to systematically find the optimum catalyst will be developed that combines the power of theory and experiment for atomistic design of catalytically active sites that through an iterative process between theory and experiment can translate the fundamental insights gained directly through this process to a complete catalyst system that can be technically deployed.

We will select simple well-defined systems for which theoretical models of 300 atoms or less can provide meaningful insights. We will initiate our work on the precious metal nanocluster catalysts on alumina and magnesia reported by Bruce Gates and his coworkers. The experimental evidence for the efficacy of catalyst will be obtained from microstructural experimental studies and catalytic testing for hydrocarbon conversion reaction and toluene hydrogenation.

Keywords: Catalytic Materials, Catalytic Testing, Experimental Catalysis

29. DURABILITY OF PARTICULATE FILTERS (CRADA WITH CUMMINS, INC.)
    $300,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

The proposed research will identify and implement test techniques to characterize the physical and mechanical properties of ceramic substrates used as diesel particulate matter filters (DPFs) and develop analysis tools for predicting their reliability and durability. The implementation of the results from this investigation will result in improved designs of more durable and reliable DPFs.

The proposed research work involves the following efforts:

Identification and implementation of test techniques to determine the strength and fracture toughness of ceramic substrates, determination of the distribution of strengths of ceramic substrate materials at various temperatures accompanied by 100 percent fractography, determination of the resistance of ceramic substrates to thermal shock, determination of the resistance of ceramic substrates to slow-crack growth in relevant environments, and implementation of a probabilistic strength design analysis to predict the durability and reliability of DPFs.

Keywords: Diesel Particulate Filters, DPFs, Ceramic Substrates

30. ADVANCED MATERIALS FOR LIGHTWEIGHT VALVE TRAIN COMPONENTS
    $100,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Caterpillar Contact: Jeremy Trethewey, 309-578-0056

The objective of this effort is to design and fabricate engine valves from high temperature advanced materials that are 30 percent lighter than steel valves, provide a 200 percent increase in service lifetime, and at least a 5 percent increase in fuel efficiency.

The selection and mechanical characterization of lightweight silicon nitride and titanium aluminide advanced materials has been completed. Probabilistic designs of 3400 and 3500 series engine valves will be made using life prediction algorithms such as NASA's CARES/LIFE and Honeywell's CERAMIC and ERICA computer codes.

Caterpillar engine manufacturing facilities that will adopt these technologies will review the proposed valve designs before having the first of two phases of prototype valves fabricated. The valves will be subjected to a variety of proof tests on an existing bench rig to assess impact, wear, and overall component reliability. The prototype valves will be sent to Argonne National Laboratory for state-of-the-art nondestructive evaluation before and after bench testing. Some of valves will be destructively tested before and after bench tests in order to assess any strength degradation processes. Probabilistic models of the prototype valves will be compared to the actual valve performance observed from the bench tests and rig. A second series of prototype valves will be fabricated based on the results of the first phase design and scheduled for engine and field tests.

Keywords: Valves, Diesel Engines, Life Prediction

31. ENGINEERED SURFACES FOR DIESEL ENGINE COMPONENTS
    $40,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Caterpillar Contact: Brad Beardsley, 309-578-8514

Engine testing of thermal sprayed coatings has demonstrated their use as thermal barriers and wear coatings can reduce fuel consumption, reduce wear and reduce component temperatures. Increase in NO_x with higher operating temperature has reduced the emphasis on insulating of the combustion chamber however reducing heat rejection through exhaust ports and manifolds remains a high priority. New approaches to thermal barrier coating design and fabrication using current phosphate bonded materials are being evaluated for these applications. Surface treatments using new wear materials for wear and friction reduction are also under development such as new quasicrystalline materials and micro-engineered powders of carbides and nitrides. Coating of these materials will be evaluated for ring and liner applications and as low friction coatings for camshafts and crankshafts. Plasma spraying, D-Gun and HVOF processing with the micro-engineered powders will be used to develop these new coatings.

Keywords: Thermal Barrier Coatings, TTBC, Plasma Spraying

32. CERMET MATERIALS FOR DIESEL ENGINE WEAR APPLICATIONS
    $100,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Cummins Contact: Randy Stafford, 812-377-3279

Earlier work at Cummins on cermet composites for wear applications produced encouraging data for several compositions of titanium carbide-nickel aluminide and tungsten carbide-cast iron materials. This data showed that the TiC/Ni_3Al had sliding wear properties near magnesia stabilized zirconia and the WC/cast iron had sliding wear properties better than conventional hardened steel and cast iron. The advantages shown by the cermet are the ability to produce a near net shape component, machinability by electrodischarge machining (EDM) and reduced wear of the counterface. An additional advantage of the WC/cast iron is potential for low cost components.

The program proposed is a follow-on to the previous work and will focus on optimization of the compositions and microstructures and evaluation of the materials from multiple production batches. The work on TiC/Ni_3Al will concentrate on one composition with up to 10 batches of powder manufactured (approximately 1 kg batch size), followed by characterization of the powder and pressing and sintering of test bars. The density, strength, and wear properties will be compared for each batch.

The work on WC/cast iron will include: optimizing the volume fraction of WC and developing a robust preform for casting and optimizing the cast iron matrix hardness and toughness (trials with grey iron and ductile iron material).

Keywords: Tribology, Wear, Cermet

33. MECHANICAL CHARACTERIZATION
    $75,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    NCA&T Contact: Jag Sankar, 336-256-1151

Task 1- Nanoengineered 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.

a. Synthesis and Mechanical Properties of TiN-AlN Thin Film Heterostructures

   There is a growing research interest in TiN and AlN due to their promising mechanical, electronic and optoelectronic properties. Our preliminary studies have shown that mechanical properties can be improved by forming thin film heterostructures of the two materials. We will explore the laser deposition assisted synthesis and perform microstructural characterizations and mechanical properties of TiN/AlN multi-layer structures.

b. Nanoengineered $Ni\text{-}Al_2O_3$ Thin Film Composite

   Nanoengineered metal-ceramic thin film composites have attracted the research attention in the recent days due to the improved structure, magnetic and mechanical properties obtained by embedding nanomagnetic particles into the ceramic matrix. Embedding of Ni metal particles into ceramic matrix should increase hardness, modulus, and fracture toughness of Al_2O_3 thin films. We will explore the development of nanoengineered ductile ceramic composites by controlling various processing parameters in PLD.

Task 2 - Solid Oxide Thin Film Electrolytes for Fuel Cell

NCA&T will continue to develop and improve the liquid-fuel-combustion CVD technique for solid oxide thin film deposition. The processing parameters for yttria stabilized zirconia (YSZ) will be optimized for best performance of these thin films in solid oxide fuel cells (SOFCs). We will also conduct research related to controlling grain size (nano to micron grain size) to observe the effects on fuel cell materials property. We will initiate both process optimization techniques and stochastic evolution model for grain growth in YSZ films with columnar microstructures. Further, enhancement of solid oxide thin film growth rate in CCVD will be investigated.

Keywords: Thermal Barrier Coatings, Nanomaterials, Thin Films, Fuel Cells

34. NDE OF DIESEL ENGINE COMPONENTS
    $200,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    ANL Contact: J. G. Sun, 630-252-5169

The purpose of this work is to characterize subsurface defects and machining and operation damage in structural ceramic valves for diesel engines using various nondestructive evaluation (NDE) methods. The primary NDE method to be addressed is elastic optical scattering or laser scattering. The goal is to demonstrate that data produced by this method can be correlated to defects/damage as well as used for predicting material microstructural and mechanical properties. There are two tasks to be completed: 1) characterize surface/subsurface defects and machining damage and correlate NDE data with mechanical properties for flexure-bar and cylindrical-rod specimens of several candidate silicon nitrides selected for valves; 2) assess/evaluate accumulated damage in full-size ceramic valves due to rig or engine tests. This proposed work is a cooperative program with Caterpillar Inc.

Keywords: NDE, Nondestructive Evaluation, Ceramic Valves

35. DURABILITY OF DIESEL ENGINE COMPONENT MATERIALS
    $200,000
    DOE Contact: James Eberhardt, 202-586-9837
    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. The approach involves test method development and use, 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, that effort was extended to include an investigation of the scuffing of fuel injector component materials. Testing techniques were developed to replicate the fine-scale surface damage that is observed in diesel engine fuel system parts. In FY 2003, the effects of sulfur content in the diesel fuel on scuffing were evaluated, and tests were conducted to evaluate the scuffing behavior of intermetallic alloy-containing cermets and traditional hard coatings in fuel environments. A new technique was developed to detect the early stages of scuffing. It is based on digitally processed friction force data, captured as a function of time. In addition, contact damage evolution in ceramics and metals for high-temperature scuffing applications was evaluated using a state-of-the-art scanning acoustic microscope. In FY 2004, multi-dimensional, graphical depictions will be created to identify combinations of surface finish and other applied contact conditions that induce mechanistic transitions to scuffing in boundary-lubricated cermets and other advanced materials. An analytical model for selecting materials for scuffing-critical applications will be developed and subsequently validated.

Keywords: Tribology, Friction and Wear, Scuffing

36. LIFE PREDICTION OF DIESEL ENGINE COMPONENTS
    $100,000
    DOE Contact: James Eberhardt, 202-586-9837
    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 in oxidative and corrosive environments. The implementation of components fabricated from these advanced materials would lead to significant improvement in engine efficiency and long-term durability and reduction in NO_x and CO exhaust emission as required in the 21st Century Truck Program. This interest has 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

37. LOW-COST MANUFACTURING OF PRECISION DIESEL ENGINE COMPONENTS
    $165,000
    DOE Contact: James Eberhardt, 202-586-9837
    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. Although ORNL has been actively involved in the development and testing of ceramic diesel engine components, an in-house machining capability currently does not exist. A process for fabricating silicon nitride valves for use in a diesel engine will be developed and demonstrated on the instrumented Weldon cylindrical grinder.

ORNL will continue to help lower manufacturing costs by collaborating with diesel engine manufacturers and machine tool manufacturers. One means of achieving cost savings is to improve the performance of consumable supplies such as coolants and abrasive wheels that are needed to produce precision engine components.

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

38. ADVANCED MACHINING AND SENSOR CONCEPT
    $100,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Univ. of Michigan Contact: Albert Shih,
    919-515-5260

The development of NO_x and particulate aftertreatment technology for diesel engines has generated the need for accurate, non-contact, and fast response temperature measurement methods to gain better insight of the chemical reactions, such as the burning of the trapped particulate or the storage and release of NO_x. A sapphire fiber with beveled tip is inserted into the cavity in the filter to harness the infrared signal to a semiconductor-based sensor. The PbS/PbSe type of sensor has successfully been tested for single-color and two-color thermal radiation temperature measurement in the 100 to 400°C range for catalyzed filters. The application of wide-band, single-color Si sensors will be evaluated for diesel exhaust filter temperature measurements. Another goal of this project is to examine the spatial and temporal temperature distribution in the diesel exhaust aftertreatment filters. A calibration method using an Inconel blackbody cavity has been developed and will be refined to improve the accuracy of measured temperature. Collaborators in this project are the Industrial Ceramic Solutions at Oak Ridge, TN, and Cummins Technical Center at Columbus, IN. One of the PhD students, Jian Kong, is expected to further develop and disseminate the experimental infrared-based temperature measurement apparatus at Cummins Technical Center in 2003-2004.

Titanium, a lightweight structural material, has been known as a difficult-to-machine and difficult-to-join material due to the low thermal conductivity and severe diffusion wear in the tools. This project develops new models and conduct preliminary experiments for friction stir welding and machining of titanium alloys. The tool wear mechanism and newly developed tool materials and PVD coatings for titanium processing will be investigated. The collaborator in this project is Kennametal Technical Center.

Keywords: EDM, Temperature Measurement, Titanium

39. ADVANCED CAST AUSTENITIC STAINLESS STEELS FOR HIGH-TEMPERATURE EXHAUST COMPONENTS
    $160,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

The objective of this new, follow-on CRADA project is commercial scale up of the new modified cast austenitic stainless steels developed by Caterpillar and ORNL as cost-effective high-performance alternatives to the standard SiMo ductile cast iron used for most diesel engine exhaust manifold and turbocharger housing components. Cast austenitic stainless steels can withstand prolonged exposure at temperatures of 750˚C or above, and are much stronger than SiMo cast iron above 550-600ºC. The new modified stainless steels (CF8C Plus and CN12 Plus) have better aging resistance and ductility after creep than standard commercial grades of the same steels. Such data forecasts better fatigue and thermal fatigue resistance than commercial cast stainless steels, and much better than SiMo cast iron, which provides resistance to cracking during the severe thermal cycling that exhaust components experience. Last year this project produced the first scale-up commercial heats of CF8C-Plus and CN12-Plus, and the CF8C-Plus is as strong as CN-12, and yet has the high ductility of standard CF8C. The initial tensile data indicates the scale-up heats behave as well or better than the earlier lab-scale heats, and the CF8C-Plus has much better fatigue resistance than CN12 steel at 700-800ºC. Testing at ORNL and Caterpillar will continue to provide the more comprehensive properties data needed by designers to qualify these new alloys, and optimize component designs. Long-term aging, creep testing, microcharacterization analysis, and casting of additional commercial heats of CF8C-Plus are underway or planned. This 2nd advanced diesel engine CRADA (Cooperative Research and Development Agreement) project (ORNL02-0658) began on July 21, 2002, and will last at least three years. More detailed information on this project must be requested directly from Caterpillar, Inc.

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

40. TiAl NANOLAMINATE COMPOSITES
$75,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
LLNL Contact: Luke Hsiung, 925-424-3125

This research-operating plan 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

41. SYNTHESIS OF POWDERS FOR TITANIUM CARBIDE/NICKEL ALUMINIDE CERMETS
$0
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
University of Colorado Contact: Alan Weimer, 303-492-3759

The overall objective of this project is to develop a rapid reaction process for the manufacture of submicron sized TiC/nickel aluminide (NiAl, Ni_3Al) cermet intermetallic powders at low cost. The manufacture of such powder has been demonstrated, however, large quantities of this powder need to be produced for sintering and part evaluation at ORNL to compare with commercially available materials.

Key tasks (FY04) for continued process development includes: 1) scale-up of the rapid reaction process to supply 500 grams of submicron TiC/Ni_3Al powder to ORNL for sintering and part evaluation (cermet intermetallic powders independently characterized at CU) and 2) scale-up of the rapid reaction process to supply 200 grams of submicron TiC powder to ORNL for their internal processing with Ni and NiAl for sintering and part evaluation (TiC powder independently characterized at CU).

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

42. LASER SURFACE TEXTURING OF LUBRICATED CERAMIC PARTS
$50,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832

The objective of this effort is to determine the effectiveness of a promising, new surface engineering approach of using regular patterns of micro-scale dimples to reduce the friction of liquid-lubricated ceramic surfaces. Surface Technologies Ltd. has developed a laser-based method to prepare surfaces with arrays of microscale dimples, typically ~120mm in diameter and several mm deep, spaced in rows about 100-200mm apart.

The need to enhance the efficiency of diesel engines, while enabling them to meet requirements for emissions, raises both engine design and materials issues. Reducing the frictional losses in engines can be achieved through one or more of the following strategies: a) redesign engine components, b) improve lubricant chemistry, c) improve methods of lubricant filtering and delivery, d) reduce churning losses in fluids, e) change the operating conditions of the engine, f) substitute more durable, low friction materials, and g) change the microscale topography of contact surfaces. This project specifically addresses the last approach. In FY 2002-3, tests were conducted to examine the efficacy of laser-produced dimples on the frictional characteristics of transformation-toughened zirconia (TTZ) and silicon carbide Hexaloy SA (SiC) sliding against silicon nitride. In addition, detailed microstructural examination and characterization of the dimpled regions was performed by a variety of techniques to evaluate the effects of the laser-dimpling process on subsurface cracking or phase transformations. In reciprocating tests, it was found that dimpling reduced friction only under well-aligned contacting conditions and at higher rates of sliding. Not all experimental results indicated improvements in friction from laser dimpling. In FY 2004, the functionality of laser dimpling will be compared with other ways to produce surface micro-topographic changes. Microstructural characterization of laser surface processed ceramics will continue, as will additional friction experiments using lubricants that vary in viscosity.

Keywords: LST, Laser Surface Texturing

43. LOW COST TITANIUM FEEDSTOCK CONSOLIDATION PROCESS
$90,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
Dynamet Technology Contact: Stanley Abkowitz, 781-272-5967

Dynamet will evaluate Ti-6A1-4V alloy billet feedstock manufactured using a combination of titanium alloy powder blended with inexpensive titanium alloy fine turnings. The blended alloy powders plus turnings will be consolidated to high density billet by isostatic pressing, vacuum sintering and hot isostatic pressing. The alloy billets will be subsequently: a) cast to test bar and evaluated, b) forged to test bar and evaluated and c) extruded to test bar and evaluated with respect to microstructure and physical and mechanical properties.

Keywords: Titanium, Powder Metallurgy

44. HIGH DENSITY INFRARED SURFACE TREATMENT OF MATERIALS FOR HEAVY-DUTY VEHICLES
$70,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832

High Density Infrared (HDI) technology is being used to produce wear and corrosion resistant coatings on iron-based materials for heavy-duty vehicle applications. In most cases, the need for wear resistance, or corrosion resistance, or high strength is only necessary in selected areas of the part that is exposed to the working environment or under high stress. Therefore, it would be desirable to use materials that are lighter or less expensive for the bulk of the part and only have the appropriate surface properties where required. Coatings based on hardmetal compositions applied onto iron-based parts appear to have the best potential for use in heavy-duty vehicles. The activities for FY 2004 will be involved with optimizing the HDI processing parameters for coating adherence, dimensional control, and desired microstructure/phase development. Parameters to be examined include power level, scan speed, preheating effects, pulsed power effects (as compared to scanning at constant power), blanket atmosphere type, and multiple scans effects (as compared to a single scan at high power). The effects of the different processing parameters on the coatings as well as the substrate properties will be determined.

Keywords: Infrared Processing, Surface Treatment

45. HIGH TEMPERATURE ALUMINUM ALLOYS
$50,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
Cummins Contact: Randy Stafford, 812-377-3279

Task 1 is a ternary phase aluminum alloy utilizing rare earth metals to provide precipitate size control and stability.

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

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

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

Keywords: Aluminum, Creep, Low-Cycle Fatigue

46. TITANIUM ALLOYS FOR HEAVY- DUTY VEHICLES
    $100,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

Titanium alloys are approximately 40 percent lighter than steel and about 36 percent lighter than cast iron. In addition, they have excellent corrosion resistance and high strengths at elevated temperatures. These properties make Ti attractive where weight and/or high performance are a requisite for a structural metallic material. This project will explore the possible uses of a wrought and/or cast Ti alloy for use in heavy-duty vehicles. The most likely uses are in the diesel engine for heads and/or blocks, connecting rods, cam shafts, crank shafts, turbocharger, and valve-train components.

Keywords: Titanium Alloys, Ti Alloys in Diesel Engines

47. MECHANICAL BEHAVIOR OF CERAMIC MATERIALS FOR HEAVY DUTY DIESEL ENGINES
    $300,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

The application of more ceramic components in engines and transportation systems would be enabled if they could be confidently manufactured and machined faster (i.e., more cost-effectively) and if mechanisms that limit their mechanical performance were understood, predictable, and controlled. This project quantifies "plasticity/fracture thresholds" in ceramics (e.g., cubic oxides and non-oxides, nanoceramics and nanocermets, piezoelectric ceramics, micaceous ceramics, and traditional structural ceramics) and examines the competing mechanisms that dictate when and how plasticity or fracture dominates the other during controlled and instrumented static and dynamic indentation and scratch testings. Special specimen preparation techniques and specialized microstructural characterization instrumentation (e.g., optical coherent tomography {OCT}, piezospectroscopy, scanning acoustic microscopy) will be used that will supplement the study and interpretation of the plastic/fracture threshold. Specific ceramics are chosen for examination because: 1) of their good potential to exhibit plasticity, or 2) their apparent plasticity is already established and therefore serves as appropriate model and reference materials for the study of plasticity fundamentals, or 3) plasticity may be potentially induced, promoted, and exploited through the concurrent application of mechanical loading and fields or other environment (e.g., temperature) or 4) they are established structural brittle materials under consideration for components in engine and transportation systems whose plasticity/fracture behavior is relevant for comparison. The thorough understanding of the competition of fracture and plasticity in ceramics will enable improved and faster means of ceramic component manufacturing and surface engineering (e.g., ductile regime machining) and maximize mechanical performance when surface condition (e.g., bending) or when surface-located events (e.g., wear, impact) are service-life-limiters in engine and transportation system components.

Keywords: Ceramic Components, Plasticity/Fracture Threshold

48. POWDER PROCESSING OF NANOSTRUCTURED ALLOYS PRODUCED BY MACHINING
    $75,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Purdue Contact: Srinivasan Chandrasekar,
        765-49-43623

Although nanostructured materials exhibit novel intrinsic property combinations, achieving their full potential in bulk components has been hampered by their high production cost and lack of processing knowledge base. Not only does the vapor phase condensation route to metal nanoparticles suffer from low production rates and limited composition control, but such fine particulate is inherently difficult to consolidate and densify by sintering due to agglomeration and contamination (e.g., oxidation). Indeed, the lack of even small bulk test specimens having well characterized nanostructure (porosity, oxides) has limited systematic studies of structure-property relationships, let alone development of bulk components.

While optimization of the process has not yet been accomplished, preliminary research has shown that nanostructured particulate of virtually any metal or alloy can be produced on a large scale by machining. The proposed scientific research focuses on fundamental processing studies aimed at establishing the basis for converting these nanostructured materials into bulk components. Both monolithic and composite forms will be developed using advanced powder processing routes, including dynamic compaction, shear-based densification, and rapid infiltration processing. A wide range of basic questions unique to the consolidation and densification of these nanostructures will be addressed systematically. Simultaneously, valuable insight into the thermal coarsening phenomena that limit the processing and ultimate performance of nanostructured materials in general will be obtained.

Keywords: Nanostructured Materials, Metal Nanoparticles

49. DEFORMATION PROCESSES FOR THE NEXT GENERATION CERAMICS
$100,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832

In addition to lower specific weight, ceramics have a number of attractive properties for application as components in various heavy vehicle systems. However, the types of heavy vehicle components require ceramics with complex shapes as well as function. Furthermore the demanding service conditions necessitate improved mechanical reliability and fracture resistance. Underlying the performance and use of ceramics is their tendency to fail in a brittle fashion except at temperatures generally well above 1000˚C. Complex shape forming processes for ceramics are relegated to approaches based on powder processing as a result of the excessive temperatures for hot forming. On the other hand, bulk metallic alloys can be hot worked at temperatures below 1000˚C to not only form the desired shape but also to enhance their properties. The ductility (> 20 percent plastic strain) of metallic alloys at temperatures below 500˚C is the source of their 10- to 100-fold greater fracture toughness as compared to that of ceramics. In ceramics systems, combined experimental and modeling studies will address approaches to reduce the temperature required for the high permanent strains (>50 percent) to be able to hot form them and to attain plastic strains of 1 to 5 percent to enhance their fracture resistance and reliability at lower temperatures. The hot forming study will extend the findings of super plastic (strains ≥ 100 percent) behavior observed in some ceramics with grain sizes (G) of > 0.1 µm to nanocrystalline (G < < 0.1 µm) ceramics. Recent studies reveal that material transport by diffusion can be greatly enhanced at temperature well below 1000˚C by forming nano-grain sized materials. This will then be combined with studies to modify the microstructure of hot-formed ceramic to develop the properties needed for specific applications. The complementary study will then address mechanisms that enable ceramics to retain some plasticity (1 to 5 percent) at temperatures well below 500˚C. This will include nanostructured ceramics to explore for the softening effects observed nanocrystalline metals and the application of external factors (e.g., electric fields) that have been shown to enhance deformation processes in ceramics with ionic bonding.

Keywords: Nanostuctured Ceramics, Nanocrystalline Ceramics

50. HIGH SPEED MACHINING OF TITANIUM
$75,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
Third Wave Contact: Kerry Marusich

Task 1 - Drilling of titanium and verification of the 3D machining model for the drilling process. The drilling process from the modeling standpoint can be divided into three stages – entry of drill point geometry into the workpiece; fully immersed cutting point geometry in the workpiece and exit of the drill point geometry from the workpiece. Process improvements in material removal rate for deep hole drilling without compromising the part quality will be investigated.

Task 2 - Face milling of titanium, with emphasis on optimized milling cutter geometry and verification of the 3D machining model for the face milling process. The validation will be done with the comparison of cutting test data of 8 different cutting conditions with variations in rake angles, lead angles and cutting conditions agreed upon between TWS and ORNL.

Task 3 - Simulation capability for boring process for machining of Ti-based automotive engine components. The simulation results will be validated with test data provided by ORNL.

Task 4 - Selection and testing of new and improved cutting tool materials that are well-suited to the machining of titanium, with emphasis on verification of the 3D machining model for the new tool materials.

Task 5 - Investigation of the use of titanium as a material for brake systems. Specifically, machining of titanium brake rotors will be investigated, with emphasis on 3D modeling of the machining process and verification of the model.

Keywords: Ti Automotive Components, Ti Drilling, Ti Face Milling, Titanium Brake Rotors

51. WALKER PROCESS FOR STRESS RELIEF
$40,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: D. R. Johnson, 865-576-6832
Acceledyne Corporation Contact: Donna M. Walker

The primary objective for this proposed research program is to validate Acceledyne's Walker Process (WP) for acceleration of both heat treatment and relief of residual stresses in crystalline materials. The secondary objective will be to demonstrate that use of the Walker Process will either leave properties unaltered or improved while reducing process time and power consumption. The process should be applicable to a wide range of materials and to any manufacturing procedure which can be described by the Arhennius first order rate equation.

Keywords: Crystalline Materials

52. SYNTHESIS OF NANOCRYSTALLINE CERAMICS
    $45,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Pennsylvania State University Contact: J. H. Adair, 814-863 6047

A research program to support one Penn State graduate student is proposed for funding through Oak Ridge National Laboratory. The graduate student will spend approximately three summer months at ORNL to conduct research on fabrication of dense, bulk nanocrystalline ceramics in addition to the time spent at the University Park Penn State campus taking required courses and conducting research.

Advanced particle processing will be used to produce dense, bulk nanocrystalline oxide ceramics. Two routes to obtaining well-dispersed powders (i.e., comminution and colloidal processing) will be emphasized. Advantage will be taken of recent advances in colloidal processing, which can result both in high green densities (> 50 percent of theoretical) with 8 nm yttria-stabilized cubic zirconia (YSZ) powders and in translucent, dense 45 nm grain sized ceramics based on preliminary sintering studies. The large surface areas of such powders lead to large quantities of adsorbates, which must be removed both to enhance particle packing and subsequent sintering. Both reactive atmosphere and microwave thermolysis have merit and will be evaluated to eliminate adsorbates at low temperatures.

Experience to date has shown that small dense nanocrystalline disks can be produced by these approaches. This project will scale-up the processes to be able to produce dense YSZ ceramics with grain sizes less than 100 nm having sample dimensions of 25 mm in diameter by 3 mm in thickness to be delivered to ORNL for further testing. Additional effort will focus on fabrication of said samples with grain sizes <50 nm for testing by ORNL staff.

Keywords: Nanocrystalline Ceramics, Nanocrystalline Oxide Ceramics

53. DEVELOPMENT OF TITANIUM COMPONENTS FOR A HEAVY-DUTY DIESEL ENGINE TURBOCHARGER
    $0
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    Caterpillar, Inc. Contact: Jeremy Trethewey, 309-578-0056

The objective of this program is to design and develop a new turbocharger for a heavy-duty diesel engine that utilizes lightweight titanium alloys for reducing transient emissions while improving engine performance.

The recent reduction in processing costs for titanium alloys makes these alloys attractive alternatives for high temperature applications in the heavy-duty diesel engine market. Caterpillar plans to make the most of these advantages in the design and development of a new turbocharger for diesel engines.

Mechanical characterization of titanium aluminide and titanium alloys will be completed to assess the strength as a function of temperature, estimate the low and high cycle fatigue resistance and toughness properties. The technologies for joining titanium aluminide to titanium alloys will be examined and a commercial viable process will be selected and optimized. A different design methodology will be used to account for the brittle and ductile behavior of titanium aluminide over the temperature range of interest. In the first phase, prototype turbochargers will be fabricated and subjected to several in-house bench tests. Engine tests of the prototype turbochargers will commence depending upon the outcome of these bench tests. A second design phase will address any shortcomings observed in the first design phase and follow with another set of prototype turbochargers fabricated. The second phase will also include bench tests but will focus mainly on completing engine tests and possibly tests in field engines.

Keywords: Turbocharger, Lightweight Titanium Alloys

54. SURFACE MODIFICATION OF ENGINEERING MATERIALS FOR HEAVY VEHICLE APPLICATIONS
    $200,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    NIST Contact: Stephen Hsu, 301-975-6120

NIST will develop a new R&D effort in the modification of engineering surfaces to improve wear and durability and to reduce friction. Surface modification will include surface texturing, such as grooves and dimples. Methods of surface modification will be evaluated, such as laser texturing, chemical etching, direct deposition, honing and grinding. Methods of surface characterization will be evaluated as well, including nanoindention, nanoscratch test, and ball-on-plane tests.

NIST will involve members of the international community in the surface modification study and, in concert with the DOE Office of Fuel Cell and Vehicle Technology (OFCVT) and the Oak Ridge National Laboratory (ORNL), will propose to the IEA-Executive Committee the formation of a new annex to study surface modification.

Keywords: Surface Modification, Laser Texturing, Chemical Etching

55. IEA IMPLEMENTING AGREEMENT FOR A PROGRAMME OF RESEARCH AND DEVELOPMENT ON ADVANCED MATERIALS FOR TRANSPORTATION APPLICATIONS
    $200,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

The International Energy Agency (IEA) was formed via an international treaty of oil consuming countries in response to the energy crisis of the 1970s. A major objective of the IEA is to promote secure energy supplies on reasonable and equitable terms. The governing board of the IEA, which is composed of energy officials from each member country, regularly reviews the world energy situation. To facilitate this activity, IEA encourages cooperation between its members countries via implementing agreements (IAs), which are the legal instruments used to define the general scope of the collaborative projects. There are currently 40 active implementing agreements covering research topics such as advanced fuel cells, coal combustion science, district heating and cooling, enhanced oil recovery, fluidised bed conversion, hydropower, heat pumping technologies, hybrid and electric vehicles, high temperature super conductivity, wind turbines, and high temperature materials. The objective of this project entitled, “Implementing Agreement for a Programme of Research and Development on Advanced Materials for Transportation Applications” 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

56. TESTING STANDARDS
    $75,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832
    NIST Contact: George Quinn

In FY 2004, work will focus on the following test methods for the American Society of Testing and Materials:

A new ASTM standard test method for flexural strength of rod specimens will be prepared.
If necessary, a small round robin may be organized within either IEA or VAMAS to confirm that different laboratories can measure rod strengths reliably. Prestandardization work will be done to refine the diametral compression (Brazilian disk) strength test method.

Keywords: Standards, ASTM, Fracture Toughness, Flexural Strength

57. IEA - ROLLING CONTACT FATIGUE
    $175,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: D. R. Johnson, 865-576-6832

The characterization and understanding of contact damage behavior of ceramics under rolling and sliding conditions are enablers to more widespread utilization of ceramics as cam followers, valves, valve seats, and other important transportation-related components. Toward that, rolling contact fatigue (RCF) studies involving both international and domestic interactions will occur in FY04. An extensive literature survey will be conducted on RCF testing in the United States and summary report will be written for exchange among the IEA Annex III participating countries (Germany, Japan, United Kingdom, and the US). Technical participants from those countries will each also compose reports and a summary report will be published that combines them all. Additionally, in serving in the capacity of the new US Technical Leader on IEA Annex III (“Cooperative Program on Contact Reliability of Advanced Engine Materials), an Annual Working Group Meeting consisting of the international participants will be organized and held in the United States to discuss mutual progress and future plans. A domestic interlaboratory comparison of RCF results on at least one commercially Si_3N_4 will be organized and technically led. Additionally, the effects (and extent) of pre-existing sub-surface damage on RCF will be examined with in a Si_3N_4. Lastly, the applicability of using acoustic scanning microscopy and optical coherent tomography to non-destructively scrutinize RCF damage in Si_3N_4 will be assessed.

Keywords: Contact Damage, IEA, Rolling Contact Fatigue

HIGH STRENGTH WEIGHT REDUCTION MATERIALS

58. APPLICATION OF INNOVATIVE MATERIALS
    $695,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: Phil Sklad, 865-574-5069
    Laboratory Partners: Oak Ridge National Laboratory
    Industry Partners: Red Devil Brakes, Caterpillar, Peterbilt

The objective of this project is to apply innovative materials in heavy vehicle components. Materials that enable weight reduction while equaling or improving performance will be identified, fabricated into prototype components, and tested. Where possible, components will be validated with full scale vehicle tests. Materials under consideration include titanium alloys and ceramic composites for heavy duty braking systems as well as novel carbon-based materials for thermal management.

Keywords: Materials, Titanium, Carbon-Based Materials, Brakes, Thermal Management

59. LIGHTWEIGHT VEHICLE STRUCTURES
    $2,765,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: Phil Sklad, 865-574-5069
    Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory
    Industry Partners: Autokinetics, DaimlerChrysler, Delphi, Freightliner, GS Engineering, Heil Trailer, International Truck and Engine, Oshkosh Truck, PACCAR, Volvo Trucks

The objective of this project is to develop lightweight materials for structural truck and bus components, develop and implement low-cost manufacturing technologies, and validate concepts on full size vehicles. Materials under consideration include aluminum, high strength steels, stainless steels, and carbon-fiber composites. Research efforts are concentrating on both body and chassis applications and are targeted on weight reductions of greater than 25 percent. This will contribute to the overall goal of a 5,000 pound reduction in the weight of Class 8 tractor trailers.

Keywords: Frames, Chassis, Manufacturing, Lightweight, Trucks, Buses

60. MATERIALS PROCESSING DEVELOPMENT
    $1,775,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: Phil Sklad, 865-574-5069
    PNNL Contact: Mark Smith, 509-375-4478
    Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Albany Research Labs, Los Alamos National Laboratory, Idaho National Laboratory
    Industry Partners: Freightliner, PACCAR, Eck Industries
    University Partners: Tennessee Technological University, University of Virginia, Ohio State University, University of Tennessee

The objectives of this project are: to develop and integrate the necessary hardware and production procedures to implement advanced casting and forming 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; to develop modeling and design capabilities for optimizing steel castings for heavy vehicle applications to reduce weight without sacrificing performance; to explore innovative forming technologies for application with lightweight metals such as magnesium, aluminum, and titanium; to explore potential advanced processing technologies for lowering the cost of carbon fiber; and to use the new processes to achieve improved microstructure, properties, performance and control in the production of components for heavy vehicles.

Keywords: Aluminum Alloy, Casting, Forming, Truck, Automotive, Aluminum Castings, Steel Castings, Magnesium, Carbon Fiber, Extrusion, Superplastic Forming

61. MATERIALS DEVELOPMENT
    $855,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: Phil Sklad, 865-574-5069
    Laboratory Partners: Oak Ridge National Laboratory
    Industrial Partners: Caterpillar
    University Partners: Brown University, University of Tennessee

The objective of this project is to develop lightweighting materials that are tailored to heavy truck applications. Activities focus on developing microstructure-level simulation tools to capture the formation and influence of nonhomogeneous microstructures in steel processing, understanding and predicting microstructural evolution, and predicting component performance. Other activities focus on titanium materials and non-conventional materials for structural applications.

Keywords: Simulation Tools, Steel, Titanium, Microstructure

62. ENABLING TECHNOLOGIES
    $2,750,000
    DOE Contact: James Eberhardt, 202-586-9837
    ORNL Contact: Phil Sklad, 865-574-5069
    Laboratory Partners: Argonne National Laboratory, National Institute for Standards and Technology, Oak Ridge National Laboratory, Pacific Northwest National Laboratory

The objective of this project is to develop technologies that support the use of lightweight materials in applications relevant to heavy vehicles. The approach is to address barriers to the implementation of these materials. Materials include aluminum, magnesium, carbon fiber composites, as well as more conventional materials such as steel and cast iron. Activities include development of cost effective technologies for joining lightweight materials as well as dissimilar materials, surface processing to enhance properties, corrosion control or mitigation, and development of low cost tooling for low volume manufacturing.

Keywords: Joining, Surface Modification, Corrosion, Friction

HIGH TEMPERATURE MATERIALS LABORATORY

63. High Temperature Materials Laboratory User Program
$6,100,000
DOE Contact: James Eberhardt, 202-586-9837
ORNL Contact: Arvid Pasto, 865-574-5123

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

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

ELECTRIC VEHICLE R&D PROGRAM

ADVANCED BATTERY DEVELOPMENT

64. NEW HIGH-CAPACITY ELECTRODES FOR LITHIUM-ION BATTERIES
$250,000
DOE Contact:Dave Howell, 202-586-3148
ANL Contact: Gary Henriksen, 630-252-4591
ANL Principal Investigator:Michael Thackeray, 630-252-9184

Argonne National Laboratory is developing new electrode materials for the next generation of lithium-ion batteries. The electrodes are activated during the initial charge process to yield high capacity metal-dioxide compounds, based predominantly on manganese and nickel. The electrode capacities are almost twice those of conventional lithium-cobalt-oxide electrodes, when operated between 4.6 and 3.0 V in lithium cells. The new electrode materials could significantly enhance the energy density of lithium-ion batteries for use in electric vehicles (EVs). Efforts are underway to improve the power capability of these electrodes for use in hybrid electric vehicles (HEVs).

Keywords: Li-Ion Battery Cathode Materials, High Capacity Li-Ion Batteries

65. NEW POLYMER STRUCTURES FOR IMPROVED LI ION ELECTROLYTES
$250,000
DOE Contact: Tien Duong, 202-586-2210
LBNL Contact: Frank McLarnon, 510-486-4636
LBNL Principal Investigator: John Kerr, 510-486-6279

LBNL has introduced a trimethylene oxide (TMO) link into polymer chains, and clearly showed that it increases the polymer mobility. However, TMO appears to lower the dielectric constant of the resulting electrolyte resulting in increased ion pairing and a decrease in the concentration of free charges to carry current. A combination of the large anions such as TFSI and BETI with TMO-containing polymers leads to better ion dissociation that, combined with increased chain flexibility, gives better transport. Future work will include investigating new polymers that offer better transport properties, and introducing butanediol groups for more flexibility and S donor atoms, developing single-ion conductor gels and dry systems, and developing polymer structures with features for 4 volt stability.

Keywords: Polymer Electrolytes for Li-ion Batteries

66. FIRST-PRINCIPLES CALCULATIONS OF IMPROVED LI-ION CATHODE MATERIALS
$220,000
DOE Contact: Tien Duong, 202-586-2210
LBNL Contact: Frank McLarnon, 510-486-4636
MIT Principal Investigator: Gerbrand Ceder, 617-253-1581

First principles calculations have been used to understand how to enhance the capacity of $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$. Computations predicted the effect of various substitutions on the voltage curve of this material. Only direct substitution of part of the Co by Fe was found to be effective, and to test this result, partially substituted materials have been synthesized. Initial electrochemical testing confirms the calculations, but also indicates poor cycling performance. The development of first-principles methods to predict electronic conductivity, in such important materials as $LiFePO_4$ and other phosphates, is underway. In addition, researchers are setting up large-scale search (computational) methods for novel cathode systems, and investigating electronic conductivity in phosphates and oxides.

Keywords: Materials Design, First Principals Calculations

67. SYNTHESIS AND CHARACTERIZATION OF CATHODE MATERIALS FOR RECHARGEABLE LITHIUM-ION BATTERIES
$340,000
DOE Contact: Tien Duong, 202-586-2210
LBNL Contact: Frank McLarnon, 510-486-4636
LBNL Principal Investigator: Marca M. Doeff, 510-486-5821

Strategies to overcome low rate capability in $LiFePO_4$ (e.g., carbon coating) often result in lowering the energy density to an unacceptably low level. Recent work (with R. Kostecki, diagnostics) is directed toward optimizing the structure of *in situ* carbon produced during $LiFePO_4$ synthesis. It has been found that small differences in processing lead to wide variations in performance. Carbons with low D/G ratios (disordered/graphene) have higher electronic conductivities and result in improved electrochemical performance, even when present in small amounts ($\leq$ 1 wt.%). In FY 2004, ways to promote formation of low D/G ratio carbon by using additives during synthesis were explored. Addition of volatile, easily decomposed pyromellitic acid (PA) and graphitization catalysts such as iron nitrate or ferrocene, results in more graphitic carbon structures on the surface and markedly improved rate capabilities of the $LiFePO_4$ samples. Future work will be directed towards determining the optimum ratio of catalyst to PA and the role of surface impurities and particle morphologies upon performance. The goal of this work is to produce high rate capability $LiFePO_4$ using minimal amounts of conductive coatings.

Keywords: Iron Phosphate Cathode Material, High Capacity Li-Ion Batteries

GEOTHERMAL TECHNOLOGIES PROGRAM

	FY 2004
GEOTHERMAL TECHNOLOGIES PROGRAM - GRAND TOTAL	$310,000
GEOTHERMAL MATERIALS	$310,000
Field Testing of Lined Heat Exchanger Tubes	100,000
High-Performance Coating Materials	90,000
Acid Resistant Cements	120,000

GEOTHERMAL TECHNOLOGIES PROGRAM

GEOTHERMAL MATERIALS

PROGRAM GOALS

The ultimate goal of the program is to develop advanced cost-effective high-temperature coating and cementitious materials that can solve corrosion, erosion, and scale deposits problems of metallic components in geothermal power plants and geothermal wells at low pH and brine temperatures up to 350˚C. These activities will result in reducing capital and life-cycle costs of metallic components along with operation cost, contributing to geothermal technologies goal of providing a more robust generation capacity along with a lower cost geothermal energy. The DOE contact is Raymond LaSala, 202-586-4198

MATEAIALS PREPARATION, SYNTEHSIS, PROCESSING, CHARACTERIZATION OR TESTING

68. FIELD TESTING OF LINED HEAT EXCHANGER TUBES
    $100,000
    DOE Contact: Raymond LaSala, 202-586-4198
    BNL Contact: Toshifumi Sugama, 631-344-4029

The objective of this program is to conduct a field validation test of 20-ft. long heat exchanger (HX) tubes lined with thermally conductive, self-healing polyphenylenesulfide (PPS) composite material being developed by BNL at Puna power plant, HI, operating at brine temperature of 200˚C, which is as much as 40˚C higher than that of the previous field tests at different plants, and then to perform post-test analyses for evaluating liner's ability to protect the underlying carbon steel tube against corrosion and to minimize irremovable scale deposits. The program also includes the assessment of the integrity and reliability of the liners fabricated using BNL-designed state-of-art lining apparatus for 40-ft.-long tubes before field tests. An ASTM non-destructive sponge holiday test is employed for this assessment. In addition, we strive to develop the optimum process technology for lining the BNL-formulated nanocomposite material that improves further the resistance to abrasive wear and enhances the hydrothermal stability for 40-ft.-long tubes. The previous field test at geothermal power plant operating at brine temperature of 160˚C demonstrated that PPS line adequately protected the carbon steel HX tubes against corrosion and fouling for more than two years, validating that this material withstood a 160˚C brine temperature and displayed a high potential for use as high-temperature anti-corrosion and –fouling liner. The components of the heat exchanger, such as tubes, shell, and sheet, are by far the major cost in a binary plant. The stainless steel and titanium alloy heat exchanger tubes presently used in such binary-cycle plants afford great protection against corrosion caused by hot brine. However, the corrosion-preventing passive oxide layers that form at the outermost surface sites of these tubes are detrimental in that the tubes become more susceptible to the deposition of silicate and silica scales, thereby developing a strong adherence to them. This strong bond not only requires using highly pressurized hydroblasting to remove these scales adhering to the tubes' surfaces, but also entails a substantial amount of time to do so. Thus, if the carbon-steel tubes could be coated with a thermally conductive material that resists corrosion, oxidation, and fouling, then the capital and maintenance costs of the heat exchanger, containing on average 800 tubes, will be markedly reduced.

Keywords: Heat Exchanger, Corrosion, Scale Deposits, Carbon Steel, Polymeric Liners

69. HIGH-PERFORMANCE COATING MATERIALS
    $90,000
    DOE Contact: Raymond LaSala, 202-586-4198
    BNL Contact: Toshifumi Sugama, 631-344-4029

The serious concerns confronting geothermal power plant operators are brine-induced corrosion, erosion, and fouling by scale deposits for the plant components such as wellhead pipes, heat exchangers, aluminum-finned condensers, and steam separators. The failure of these components causes a decrease in electrical generation, the decline of efficiency and profitability of plants, and an increase in capital and operational costs along with an environmental issue. In resolving these problems, the objectives of this program are to develop a 300°C-stable yet tough polyetheretherketone (PEEK)-based nanocomposite coating for well head pipes and heat exchangers, and to synthesize a new type of organometallic polymer (OMP) for potential use as a thin glassy coating for the condensers as well as to develop a slick, low-surface energy Teflon-based coating for steam separators. The project also was designed to obtain a fundamental understanding of the characteristics of the developed and synthesized coating systems before applying them to full-scale metal substrates. The ultimate goal of this program is to extend the useful lifetime of inexpensive carbon steel well head pipes, heat exchangers, and steam separators under a harsh, hostile environment with ³ 200˚C brine by coating them with the nanocomposite and Teflon-rich coatings, and similarly to enhance the efficacy of the condensers by applying a very thin hard coating film. The success of these coating systems will not only increase electric generation capacities, but also will save substantial capital costs because they will eliminate the need to use expensive stainless steel, titanium alloys, and inconel.

Keywords: Coatings, Corrosion, Polymer Nanocomposite, Organometallic Polymer, Teflon, Plant Components

70. ACID RESISTANT CEMENTS
    $120,000
    DOE Contact: Raymond LaSala, 202-586-4198
    BNL Contact: Toshifumi Sugama, 631-344-4029

The objectives of this task are to modify the cost-effective sodium silicate-activated slag cements developed in the previous FY with fly ash F as an industry byproduct that makes it possible to incorporate the anti-acid zeolite phase into the cement bodies, to investigate potential of air-foamed low-density calcium aluminate phosphate (CaP) cement slurry for replacing N_2 gas-foamed conventional cement slurries, and also to conduct post-field test analyses of CaP cement being emplaced by Halliburton in Coso's geothermal wells. The primary goal of this program is to formulate new type of cements with superior acid-resistant properties that show less than a 5wt% loss after 30 days immersion in 5,000 ppm CO_2-laden H_2SO_4 brine (pH < 1.1) at temperatures up to 200˚C. A secondary goal is to design an air-foamed CaP cement slurry with a density of < 1.22 g/cc and uniform dispersion of nano/micro-size fine discrete air-bubble cells. This hardened foam cement is required to posses a good adherence to steel casing and an ability to protect the casing against corrosion. The highly concentrated CO_2 and H_2S environments encountered in the upper regions of the wells (~ 3,800 ft. below the well's surface) at temperatures up to 200˚C occasioned the former research objective of acid resistance. The latter was related to dealing with the problem of lost circulation caused by circulating conventional slurry of typical density, 1.9 to 2.0 g/cc under high hydrostatic pressure. Severe acid erosion and an insufficient protection of casing against corrosion lead to downtime or even failure of the wells, and the requirement for expensive time-consuming remediation involving redrilling and recementing operations. Thus, the improved cements will not only significantly extend the useful lifetime of the well casing pipes, but also will save the substantial costs needed for the remedial operations of any damaged wells. Wells completed with the improved cement are projected to have service lifetimes of 30 years, thereby improving the efficiency and lowering the costs of energy-extracting operations at the plants.

Keywords: Calcium Aluminate Phosphate, Zeolite, Air-Foamed Cement, Acid Resistance, Geothermal Well Completion

HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM

	FY 2004
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM - GRAND TOTAL	$10,173,646
HYDROGEN STORAGE MATERIALS PROGRAM	$7,772,146
HIGH CAPACITY METAL HYDRIDES	$3,940,739
Catalytically Enhanced Complex Metal Hydride Materials for Hydrogen Storage	259,768
Hydride Development for Hydrogen Storage	1,875,000
High Density Hydrogen Storage System Prototype Using $NaAlH_4$ Based Complex Compound Hydrides	762,000
Discovery of Novel Complex Metal Hydrides for Hydrogen Storage Through Molecular Modeling and Combinatorial Methods	553,807
Complex Hydride Compounds with Enhanced Hydrogen Storage Capacity	490,164
CARBON-MATERIALS	$2,150,000
Hydrogen Storage in Nanostructured Carbon Materials	2,150,000
CHEMICAL HYDROGEN MATERIALS	$1,371,000
Chemical Hydride Slurry for Hydrogen Production and Storage	600,000
Design and Development of New Carbon-based Sorbent Systems for an Effective Containment of Hydrogen	771,000
NEW MATERIALS & CONCEPTS	$310,407
Sub-nanostructured Non-transition Metal Complex Grids for Hydrogen Storage	310,407
HYDROGEN PRODUCTION MATERIALS PROGRAM	$1,409,000
PHOTOELECTROCHEMICAL PRODUCTION OF HYDROGEN	$1,409,000
Photoelectrochemical Systems for H_2 Production	400,000
Photoelectrochemical Hydrogen Production Program	509,000
Discovery of Photocatalysts for Hydrogen Production	300,000
Photoelectrochemical Hydrogen Production Using New Combinatorial Chemistry Derived Materials	200,000
FUEL CELL MATERIALS	$992,500
Microstructural Characterization of PEM Fuel Cells	200,000
Cost-Effective Metallic Bipolar Plates Through Innovative Control of Surface Chemistry	300,000
Compact Carbon foam Radiator for Fuel Cell Power Systems	142,500
Selective Catalytic Oxidation of Hydrogen Sulfide	350,000

HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM

Hydrogen and fuel cell technologies have the potential to solve the major energy security and environmental challenges that face America today—dependence on petroleum imports, poor air quality, and greenhouse gas emissions. The DOE Office of Energy Efficiency and Renewable Energy (EERE), together with the Offices of Fossil Energy; Nuclear Energy, Science and Technology; and Science, are working to implement the President's Hydrogen Fuel Initiative and develop technologies to realize his vision of a hydrogen economy. The DOE Hydrogen Program responds to several recommendations in the President's National Energy Policy, including the development of next generation technologies, establishment of an education campaign that communicates potential benefits, and better integration of subprograms in hydrogen, fuel cells, and distributed energy. The Department of Energy is the lead Federal agency for directing and integrating activities in hydrogen and fuel cell R&D.

Guided by the National Hydrogen Energy Vision and Roadmap (available at http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/vision_doc.pdf and http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/national_h2_roadmap.pdf), the EERE Hydrogen, Fuel Cells & Infrastructure Technologies Program works in partnership with industry, academia, and national laboratories—and in close coordination with the FreedomCAR Program and other programs at the Department of Energy to:

- Overcome technical barriers through research and development of hydrogen production, delivery, and storage technologies, as well as fuel cell technologies for transportation, distributed stationary power, and portable power applications;
- Address safety concerns and develop model codes and standards;
- Validate and demonstrate hydrogen and fuel cell technologies in real-world conditions;
- Educate key stakeholders whose acceptance of these technologies will determine their success in the marketplace.

Materials research in Hydrogen, Fuel Cells and Infrastructure Technologies is performed under the Hydrogen Storage, Hydrogen Production and Delivery, and Fuel Cells subprograms.

Hydrogen storage is a key enabling technology for the advancement of hydrogen and fuel cell power technologies in transportation, stationary, and portable applications. DOE's efforts focus primarily on the R&D of on-board vehicular hydrogen storage systems that will allow for a driving range of 300 miles or more. In addition, hydrogen storage systems for off-board applications such as the hydrogen delivery and refueling infrastructure, and vehicle interface technologies for the refueling of hydrogen storage systems on vehicles are also being investigated. DOE's goal for hydrogen storage is to develop and demonstrate viable hydrogen storage technologies for transportation and stationary applications. The DOE/HFCIT contact for hydrogen storage is Sunita Satyapal, 202-586-2336.

Hydrogen can be produced from a variety of feedstocks using a variety of process technologies. Feedstock options include fossil resources such as coal, natural gas, and petroleum, and renewable resources such as biomass, sunlight and wind. Process technologies include thermochemical, biological, electrolytic and photolytic. DOE's goal for hydrogen production is to research and develop low-cost, highly efficient hydrogen production technologies from diverse, domestic sources, including fossil, nuclear, and renewable sources. The DOE/EERE contact for hydrogen production and delivery is Peter Devlin, 202-586-4905.

Fuel cells are one of the key enabling technologies for a future hydrogen economy. The have the potential to replace the internal combustion engine in vehicles and to provide power in stationary and portable power applications because they are energy-efficient, clean, and fuel-flexible. For transportation applications, DOE is focusing on direct hydrogen fuel cells, in which on-board storage of hydrogen is supplied by a hydrogen generation, delivery, and fueling infrastructure. For distributed generation fuel cell applications, the program focuses on near-term fuel cell systems running on natural gas or propane and recognizes the longer term potential for systems running on renewable fuels. DOE's goal for fuel cells is to develop and demonstrate fuel cell power system technologies for transportation, stationary, and portable applications. The DOE/EERE contact for fuel cells is Valri Lightner, 202-586-0937

HYDROGEN STORAGE MATERIALS PROGRAM

HIGH CAPACITY METAL HYDRIDES

71. CATALYTICALLY ENHANCED COMPLEX METAL HYDRIDE MATERIALS FOR HYDROGEN STORAGE
$259,768
DOE Contact: C. Read, 202-586-3152
University of Hawaii-Manoa Contact: C. Jensen

The University of Hawaii is developing catalytically enhanced complex hydride materials capable of being used in vehicular applications. The researchers have sought to gain a fundamental understanding of the nature of the dopants and the structural effects they exert on the hydride using novel material synthesis strategies and detailed structural and functional characterizations. The fundamental understanding gained from the alanate system can then be applied towards the design of other complex hydrides with higher capacities that have the potential of surpassing the DOE/FreedomCAR storage performance targets. In addition to the earlier EPR and kinetic evidence, the group has obtained IR and XRD results supporting their "substitution" model of Ti-doped $NaAlH_4$. The group has concluded from both EPR and synchrotron X-ray studies that the majority Ti species changes from Ti(III) to an AlTi alloy during the first few cycles of dehydrogenation/hydrogenation. Despite this change, only a minor change in the hydrogen cycling kinetics occurs. This would seem to suggest that the enhanced hydrogen cycling kinetics is due to a Ti species that is present in only a relatively minor amount. The slight kinetic improvement that is observed beyond the third cycle is similar to those observed when the hydride is ball milled without dopant. The finding that a significant amount of the AlTi alloy arises after the third cycle then suggests that the alloy is responsible for this minor kinetic enhancement and acts as an anti-sintering agent. The group's adoption of the "substitution" model has guided them to the preparation of "$Ti_{x/3}Na_{1-x}AlH_4$," "$Ti_xNa_1AlH_4$," and a novel complex hydride. The evaluations of the hydrogen storage performance of these materials that are currently underway will provide a true test of the validity and value of the "substitution" model of doped complex hydrides.

Keywords: Complex Hydrides, Alanates, Hydrogen Storage

72. HYDRIDE DEVELOPMENT FOR HYDROGEN STORAGE
$1,875,000
DOE Contact: C. Read, 202-586-3152
Sandia National Laboratory-Livermore Contact: J. Wang

The purpose of this project is to discover and develop the next generation of practical metal hydride hydrogen storage materials and to measure the engineering properties of their use. This work will focus on new materials including complex metal hydrides and modified amides with high reversible hydrogen storage capacities. This project has grown from a foundation of achievements that Sandia made in developing advanced Ti-doped Na-alanates. SNL has achieved 5 wt.% reversible hydrogen storage through the development of a destabilized Mg-modified Li-imide material. Using an oxide doping precursor and hydrogen-driven metallurgical reactions, metallurgical stimulated thermal H_2 desorption from $NaBH_4$ was demonstrated. Using particle size control and metallurgical stimulation, Sandia experimentally demonstrated 7-8 wt.% H_2 desorption from AlH_3 at temperatures <200˚C, i.e., demonstrated clear potential for meeting the DOE 2010 weight and volume system targets. SNL has used solution synthesis to make Li- and K-based complex hydrides. Nano-crystalline and amorphous amides and imides have been produced using solution and gas reaction synthesis. The Sandia theoretical group has used first-principles calculations and experimental work to provide new insight into the role of titanium in the hydrogen sorption mechanisms of Ti-doped alanates. Materials engineering properties (thermal conductivity, lattice expansion forces, and electrical properties) of the alanates have been characterized in detail. Sandia has installed experimental capabilities to determine durability, contamination effects, safety and special synthesis techniques.

Keywords: Complex Hydrides, Alanates, Hydrogen Storage

73. HIGH DENSITY HYDROGEN STORAGE SYSTEM PROTOTYPE USING $NaAlH_4$ BASED COMPLEX COMPOUND HYDRIDES
$762,000
DOE Contact: C. Read, 202-586-3152
United Technologies Research Center Contact: D. Anton

This project is focusing on the reversible complex hydride, $NaAlH_4$, with a theoretical hydrogen capacity of 5.5 wt%, and seeks to enhance the material for improved charging and discharging rates as well as increased hydrogen capacity. The project also seeks to apply this material in the development of a prototype system which will reversibly store a high wt% of hydrogen at low pressure for an indefinite amount of time. The design of the system is also meant to be flexible towards using similar behaving complex hydrides in addition to sodium alanate. The storage system which contains the complex hydride powder must serve two primary functions: 1) exchange heat between the powder and a working liquid to drive the absorption/desorption of hydrogen; 2) support elevated hydrogen pressure during refueling. These functions must be performed with a minimum of weight, volume and cost. Numerous experiments were carried out on catalyzed $NaAlH_4$ in various phases of decomposition. The results indicate these materials to be flammable when in contact with water or water vapor in the air. The partially discharged material containing a mixture of Na_3AlH_6 and aluminum powder was found to be somewhat more reactive than the fully charged material, but in all cases, the packing classification did not change. Significant advances have been made in modeling of the media utilizing a combination of atomistic and thermodynamic methods. If the catalytic additions can made to stay within the host structure upon repeated sorption cycles, the full 5.5 wt% of hydrogen should be accessible at pressures above 1 bar. Kinetic modeling of a new catalyst type with associated processing methods holds promise of lowering the charging pressure while increasing charging and discharging rates. System designs have been completed and projections made as to the gravimetric and volumetric density of prototype generation 1. It is projected that improvements to the current catalyst compositions and system designs will be required to meet future DOE goals.

Keywords: Complex Hydrides, Alanates, Hydrogen Storage

74. DISCOVERY OF NOVEL COMPLEX METAL HYDRIDES FOR HYDROGEN STORAGE THROUGH MOLECULAR MODELING AND COMBINATORIAL METHODS
    $553,807
    DOE Contact: C. Read, 202-586-3152
    UOP LLC Contact: D. Lesch

Recently, it has been shown that the complex hydride NaAlH4 can reversibly absorb hydrogen at lower pressures and temperatures than MgH2 and has a higher gravimetric capacity and lower cost than LaNi5H6. Complex hydrides form a new class of reversible hydrides which have not been fully explored. This project proposes to systematically survey complex hydrides to discover a material which would enable a hydrogen storage system that meets DOE's 2010 goals. The team will apply methods of combinatorial chemistry and molecular modeling to discover materials with optimum thermodynamics and kinetics for on-board hydrogen storage. The increased throughput of combinatorial methods enables many more materials and conditions to be investigated for systematic study of the trade-offs between storage capacity and stability. Virtual high-throughput screening (VHTS) exploits the capability of molecular modeling to estimate the thermodynamics on the computer more quickly than can be measured in the laboratory. VHTS will be used to screen complex hydrides to find materials which could meet the DOE system requirements and focus the synthesis effort on making the most promising materials. Even more importantly, the coupling of combinatorial experiments with molecular modeling of structural and thermodynamic properties will provide insights into the underlying mechanisms of action in these complex materials, permitting the design of hydrogen storage materials which would never have been envisioned otherwise.

Keywords: Complex Hydrides, Molecular Modeling, Combinatorial Chemistry

75. COMPLEX HYDRIDE COMPOUNDS WITH ENHANCED HYDROGEN STORAGE CAPACITY
    $490,164
    DOE Contact: C. Read, 202-586-3152
    United Technologies Research Center Contact: D. Anton

The objective of this project is to explore the quaternary phase space between sodium hydride (NaH), aluminum hydride (AlH_3), transition metal or rare earth (M) hydrides (MH_z, where z = 1-3) and molecular hydrogen (H_2) to discover new complex hydride compounds capable of reversibly storing hydrogen to a capacity of > 7.5 wt %. To aid in this work, UTRC has developed a methodology for computationally evaluating the thermodynamic stability of a wide range of possible structures having high hydrogen capacity. The group will determine the optimum synthesis route for obtaining stable compounds from: 1) solid-state processing, 2) molten-state processing or 3) solution-based processing. For the most promising phases, the team will characterize the structures; demonstrate the operable temperature and pressure range of these compounds and the sorption kinetics under various conditions; determine the cyclic stability of these compounds and determine the economics of scaling up these materials to full production. UTRC has used atomistic & thermodynamic modeling to predict thermodynamic stabilities of various structures in the $Na_iTi_jAl_kH_x$ system. Solid-state processing has been used to characterize the $Na_iTi_jAl_kH_x$, $Na_iLi_jAl_kH_x$ and $Na_iMg_jAl_kH_x$ systems at 200 bar and temperatures ranging from 80 to 120˚C. A quantitative x-ray diffraction assessment has been carried out on this material with an understanding of the various phase relationships identified. Molten-state processing has been used to characterize the $Na_iK_jAl_kH_x$ system. Initial trial runs have been completed using solution-based processing in the $Na_iTi_jAl_kH_x$ system.

Keywords: Complex Hydrides, Hydrogen Storage

CARBON-MATERIALS

76. HYDROGEN STORAGE IN NANOSTRUCTURED CARBON MATERIALS
$2,150,000
DOE Contact: S. Satyapal, 202-586-2336
National Renewable Energy Laboratory (NREL)
Contact: M. Heben

The long-term goal of the project is to enable efficient adsorption of hydrogen at ambient temperature and pressure on nanostructured carbon materials. Nanostructured carbon materials have shown tremendous promise for breakthrough performance in many laboratories around the world, yet the capabilities of these materials remain controversial due to poor reproducibility in sample preparation and measurement. In addition to developing materials to meet DOE targets, the major focus of this project in FY04 was on reproducibility. This objective is in line with making a Go/No-Go decision on single-walled carbon nanotubes (based on achieving 6 wt.% storage capacity) by the end of FY06. The successful development of carbon materials for hydrogen storage will require: 1) a detailed understanding of the mechanisms that give rise to adsorption interactions in the range of 20-40 kJ/mol; 2) methods to fabricate materials having a high gravimetric density of sites displaying such interactions; and 3) approaches to arrange these sites in space to enable high volumetric storage densities. Pure carbon SWNTs and SWNT-hybrid materials remain prime candidates for development because these materials can be formed into well-packed nanoporous solids and have electronic properties that may be controlled through nanotube geometry, the introduction of defects, attachment of electronic species, elemental substitution on the nanotube lattice, and the introduction of adventitious dopants or catalytic species. Other nanostructured carbon materials such as nanohorns, multi-wall nanotubes (MWNTs), and metal oxide frameworks (MOFs) are also of interest because they provide additional systems in which adsorption interactions with hydrogen may be investigated and controlled. Hydrogen uptake values for alloyed SWNTs as reported by the NREL team during peer review were deemed credible. NREL’s TPD and volumetric techniques were demonstrated to be accurate and repeatable based on a reference standard and showed excellent correlation between techniques using similar samples. Large variances in H_2 uptake for SWNT materials are not related to analytical methodologies; they are likely due to the stochastic nature of sample processing (synthesis, purification, cutting, dopant uptake). Variances may also be related to the sensitivity of samples to degradation during the degas cycle. TPD measurements and computational modeling show the binding energy of multi-wall carbon nanotubes with Fe nanoparticles at their tips to be ~50-55 kJ/mol, which is in the range between simple physisorption and chemisorption. A definite improvement in the reproducibility and an increase in the observed H_2 storage capacity to 3 wt.% have been made.

Keywords: Carbon Nanotubes, Hydrogen Storage

CHEMICAL HYDROGEN MATERIALS

77. CHEMICAL HYDRIDE SLURRY FOR HYDROGEN PRODUCTION AND STORAGE
$600,000
DOE Technology Development Manager:
S. Satyapal, 202-586-2336
Safe Hydrogen, LLC Contact: A. McClaine

Chemical hydride slurry provides a promising means for storing, transporting, and producing hydrogen. As a pumpable medium, it can be metered and transported within the existing liquid fuel infrastructure. The chemical hydride slurry has a high energy density on a material basis (twice the volumetric energy density of liquid hydrogen and 11.7% hydrogen by mass). When hydrogen is needed, the chemical hydride slurry is metered into a chemical reaction vessel with water. The spent hydroxide slurry is returned to a large recycle plant in the vehicles that originally delivered the hydride slurry. At the recycle plant, the hydroxide is separated from the slurry oils, it is reduced to metal, the metal is hydrided to the original chemical hydride, and the chemical hydride is incorporated into new slurry using the original oils. In addition to use for on-board vehicular storage, the proposed approach may be even more applicable to off-board storage systems, where there are fewer constraints for the additional weight and volume for the water reactant. This project has been designed to define the characteristics and costs associated with a MgH_2 slurry system. The project is focused on three areas: the development of a stable, pumpable MgH_2 slurry and the design of the process required to make the slurry; the development of a simple, compact, and light mixer system to produce hydrogen from the reaction between MgH_2 and water; and the development and definition of the processes required to recycle the byproducts of the reaction back to MgH_2 slurry. The recycle process involves several steps: the hydroxide must be separated from the slurry oils and reduced to metal; the metal must be hydrided; and the metal hydride must be incorporated into new slurry. Tasks have been defined to address each of the subsystem designs. Each process will be analyzed to estimate the capital and operating costs that are likely to be required for large-scale application of the process.

Keywords: Chemical Hydride Slurry, Hydrogen Production, Hydrogen Storage

78. DESIGN AND DEVELOPMENT OF NEW CARBON-BASED SORBENT SYSTEMS FOR AN EFFECTIVE CONTAINMENT OF HYDROGEN
$771,000
DOE Technology Development Manager:
S. Satyapal, 202-586-2336
Air Products and Chemicals, Inc. (APCI) Contact:
A. Cooper

Air Products is developing liquid-phase hydrogen storage materials ("liquid hydrides") that can be reversibly hydrogenated, allowing the storage of hydrogen in a safe, easily transportable form. The liquid hydrides can be hydrogenated at large central or regional sites in locations where inexpensive hydrogen is available. Hydrogenation in an industrial facility allows for maximum overall energy efficiency through recovery and use of the heat generated by the exothermic hydrogenation. The hydrogenated liquid hydride could be distributed, using the existing liquid fuels infrastructure, to distribution sites where the liquid would be dispensed to hydrogen-powered vehicles. Onboard a vehicle powered by a hydrogen fuel cell (FC) or hydrogen internal combustion engine (ICE), the liquid would pass through heat exchanger(s) and catalyst to release hydrogen and deposit the "spent" carrier into a separate tank. The amount of waste heat available from either a FC or ICE is sufficient to supply the necessary energy for the endothermic dehydrogenation reaction. A liquid-phase hydrogen carrier has been identified which provides a >5.5 wt. % H_2 and >50 g H_2/L capacity operating in a temperature/ pressure swing mode. The carrier provides a flow of H_2 at ca. 1 atm at <200˚C, much milder conditions than reported for liquid carriers of the prior art. The APCI liquid-phase hydrogen carriers can be regenerated (most likely off board vehicles) by a direct catalytic reaction with hydrogen. Solid-state, carbon-based compositions have been identified which also function as temperature/pressure hydrogen carriers in the presence of suitable catalysts. However, their hydrogenation/dehydrogenation rates are slower than the above liquid system. Novel, carbon-based, ionic solid compositions have been identified that, by quantum mechanics/molecular dynamics calculations, show interaction energy with molecular hydrogen, a property that could render them useful as hydrogen carriers.

Keywords: Liquid Hydrides, Carbon-Based Sorbents, Hydrogen Storage

NEW MATERIALS & CONCEPTS

79. SUB-NANOSTRUCTURED NON-TRANSITION METAL COMPLEX GRIDS FOR HYDROGEN STORAGE
$310,407
DOE Technology Development Manager: C. Read,
202-586-3152
Cleveland State University Contact: O. Talu

One major problem with metal hydride systems is the slow kinetics of hydrogen uptake/release due to two reasons: 1) intrinsic reaction rate of the hydrogen molecule dissociation on the external surface of the metal, and 2) slow diffusion of atomic hydrogen in the dense metal phase. In this project, Cleveland State proposed to grow sub-nanostructured metal grids (about 1 nm metal thickness) with about 50% micro-porosity (pores about 1 nm wide). The grids are proposed to increase the overall hydrogen dissociation reaction rate (since the external metal area is enhanced) and to decrease the diffusion time constants (since the diffusion path is greatly reduced). In addition, it is proposed that the high mass transfer rates through the pores will enhance the heat transfer. The flexibility of such a grid is expected to lower decrepitation caused by cycling. Hydrogen storage capacity may also increase due to contributions by physical adsorption and through possible quantum effects. The nanostructured metal grids will be grown from pure and alloyed non-transition metals. The physical properties will be characterized by imaging (HRTEM, STEM, SEM, AFM, and STM) and by density, thermal conductivity, and electrical resistivity measurements. The metal hydride phase diagram will be measured (P-T behavior). The phase diagrams are expected to be different from the bulk phase diagrams because of the quantum effects that may arise at these length scales. In addition, the hydrogen uptake/release rate data will be collected. These measurements will enable a complete evaluation of these novel metal grids for hydrogen storage application. These nanostructured metal grids are expected to provide significant performance advantage over the same metals in bulk form. The technical approach can be summarized in three steps: 1) Coat a cathode with zeolites to act as template; 2) Employ electrochemical deposition of metal cations in zeolite pores to grow subnanostructured metal grids; and 3) Dissolve zeolite mold, leaving the metal grid only. This approach is generically applicable to any pure or mixed metal system, although the electrochemistry is considerably complicated for electrodepositing metal mixtures. Pure metals (e.g. copper, nickel, titanium) are being used in initial experiments for proof of concept. First hydrogen storage testing will be performed with palladium.

Keywords: Nanostructured Metal Grids, Hydrogen Storage

HYDROGEN PRODUCTION MATERIALS PROGRAM

PHOTOELECTROCHEMICAL PRODUCTION OF HYDROGEN

80. PHOTOELECTROCHEMICAL SYSTEMS FOR H_2 PRODUCTION
    $400,000
    DOE Contact: Roxanne Garland, 202-586-7260
    National Renewable Energy Laboratory Contact:
    John A. Turner

Direct conversion systems combine the capture of solar light energy with a water splitting system with the goal of producing hydrogen in a single step; water is split directly upon illumination with no external electron flow. An illuminated semiconductor immersed in aqueous solution—termed a photoelectrochemical, or PEC, system—exemplifies such a direct conversion system. Light impinging on the semiconductor material generates an internal electric field within the material and water can be split, with hydrogen (for example) being generated at the illuminated surface and oxygen being generated on the back (dark) side. These PEC systems have been a focus of a number of researchers for over 30 years. One of the major advantages of these PEC systems is that they operate under direct solar light. At solar intensities, the effective current density that is generated at the surface is 10-20 mA/ cm^2, depending on the type of material used. At these current densities, the energy required for electrolysis is much lower than that for commercial electrolyzers, and therefore, the corresponding electrolysis efficiency is much higher. At a current density similar to short circuit photocurrent from a solar cell, hydrogen and oxygen generation is achieved at an applied voltage of approximately 1.35 V, giving rise to an electrolysis efficiency of 91%. This then is one of the advantages of a direct conversion hydrogen generation system; not only does it eliminate most of the costs of the electrolyzer, it also has the possibility of increasing the overall efficiency of the process.

PEC hydrogen production is in an early stage of development and depends on a breakthrough in materials development. The primary effort in this project is to synthesize a semiconducting material or a semiconductor structure with the necessary properties. For the direct PEC decomposition of water to occur, three key energetic conditions and the criteria of stability for the semiconductor must be met. For the energetic conditions, the semiconductor's band gap must be sufficiently large to split water and yet not too large as to prevent efficient absorption of the solar spectrum (ideally 1.8-2.2 eV), the band edges of the semiconductor must overlap the hydrogen and oxygen redox potentials, and the charge transfer across the semiconductor/liquid interface must be fast enough to prevent band edge migration. In addition, the semiconductor's surface must be stable against corrosion both in the dark and under illumination.

For FY 2004, NRLE's study of PEC direct conversion systems involved two areas of materials research focusing only on the issues of semiconductor band gap and corrosion resistance.

Keywords: Hydrogen Production, Photoelectrochemical

81. PHOTOELECTROCHEMICAL HYDROGEN PRODUCTION PROGRAM
    $509,000
    DOE Contact: Roxanne Garland, 202-586-7260
    Hawaii Natural Energy Institute, University of Hawaii at Manoa Contact: Eric L. Miller

The Thin Films Laboratory at the Hawaii Natural Energy Institute of the University of Hawaii (UH) has been developing high-efficiency, potentially low-cost, photoelectrochemical (PEC) systems to produce hydrogen directly from water using sunlight as the energy source. The main thrust of the PEC systems research at UH has been the development of integrated multi-junction photoelectrodes based on low-cost semiconductor, catalytic, and protective thin films. This multi-junction device combines thin-film solid-state with PEC junctions to meet the voltage, current and stability requirements for hydrogen production. The development effort has relied on continued use of integrated models for photoelectrode design [3], establishment of industry and university partners with thin-film materials expertise, and fabrication and evaluation of photoelectrode test devices.

Keywords: Hydrogen Production, Photoelectrochemical

82. DISCOVERY OF PHOTOCATALYSTS FOR HYDROGEN PRODUCTION
    $300,000
    DOE Contact: Roxanne Garland, 202-586-7260
    SRI International Contact: D. Brent MacQueen

The use of high-throughput techniques to speed the materials discovery process has been in place for a number of years, the pharmaceutical companies being the first to invest heavily into the combinatorial synthesis and high-throughput analysis concept. The key to the concept is to test as many samples as possible as quickly as possible for a specific property rather than to do a complete characterization on a specific material or class of materials. In this manner, candidates for further study can be culled from very large sample sets. In developing tools for the high-throughput screening of materials for properties relevant to PEC hydrogen production, we have designed and built a 25-cell module to analyze the photolysis products generated upon illumination of samples with a simulated solar spectrum. SRI International has investigated a number of systems with respect to photocatalytic water splitting. These systems consisted of a semiconductor nanoparticle with a transition metal—Ni, Ru, and/or Pt— deposited on the surface and immersed in an electrolyte. The particles studied to date include titanium, niobium and tantalum oxides, oxysulfides, carbides, nitrides, and ferroelectric materials.

Keywords: Hydrogen Production, Photoelectrochemical, Photocatalyst

83. PHOTOELECTROCHEMICAL HYDROGEN PRODUCTION USING NEW COMBINATORIAL CHEMISTRY DERIVED MATERIALS
$200,000
DOE Contact: Roxanne Garland, 202-586-7260
University of California Santa Barbara Contact: Eric W. McFarland

The approach of this project involves the application of combinatorial chemistry methods to discover and optimize photoelectrochemical materials and systems for cost-effective hydrogen production. This represents a shift in the research paradigm from conventional chemical research in that a combinatorial approach features systematic and high-speed exploration of new metal-oxide-based solid-state materials. By investigating large arrays of diverse materials, UC Santa Barbara is working to improve the understanding of the fundamental mechanisms and composition-structure-property relationships within these systems while discovering new and useful energy-producing photocatalysts. It should also be noted that the approach focuses upon the investigation of semiconductor materials that are inherently inexpensive, such as ZnO, WO_3, and Cu_2O. Although more expensive systems (eg., GaAs, InP, etc.) have generally demonstrated greater efficiency, cost and/or natural abundance could be problematic on a large scale; thus, we are applying combinatorial techniques toward inexpensive host photocatalysts with the aim of improving their properties significantly while negligibly affecting cost.

UC Santa Barbara has designed and developed automated electrochemical synthesis and photoelectrochemical screening systems, for a variety of new materials, and has focused primarily on WO_3 and ZnO hosts, investigating libraries of variable composition and morphology. They have also developed a general method for the production of high surface area nanostructured films (WO_3, ZnO, TiO_2, Pt) by utilizing electrochemically driven self-assembly of surfactants and a pulsed-electrodeposition scheme for depositing nanoparticulate pure metals (Pt, Au, Pd), alloys (Pt-Au, Pt-Ru) and metal oxides (WO_3).

Keywords: Hydrogen Production, Photoelectrochemical, Combinatorial Chemistry

FUEL CELL MATERIALS PROGRAM

84. MICROSTRUCTURAL CHARACTERIZATION OF PEM FUEL CELLS
$200,000
DOE Contact: N. L. Garland, 202-586-5673
ORNL Contact: T. R. Armstrong, 865-574-7996

This goal of this project is to elucidate MEA degradation and/or failure mechanisms by conducting extensive microstructural characterization of both fresh MEAs and MEAs aged under load, develop correlations between as-processed MEA microstructure and performance, and collaborate with PEM fuel cell developers/manufacturers to evaluate their MEAs using advanced electron microscopy techniques and provide feedback for MEA optimization.

In a collaborative study with Los Alamos National Laboratory (LANL), the particle sizes and distributions of aged platinum electro-catalysts (in cathode) are being quantified by using high-resolution high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) for comparison with data acquired from the same samples via X-ray diffraction (XRD). Specimens for XRD were prepared by carefully scraping the Pt/C high-surface-area support material off of the Nafion membrane from the cathode side of the MEA. The specimens for HAADF-STEM were prepared in a cross-section from the scraped MEAs by ultramicrotomy in order to retain the spatial distribution of platinum, carbon, and recast ionomer constituents within the cathode in localized unscraped regions.

Keywords: Transmission Electron Microscopy, MEAMEA, Microstructure, Aging

85. COST-EFFECTIVE METALLIC BIPOLAR PLATES THROUGH INNOVATIVE CONTROL OF SURFACE CHEMISTRY
$300,000
DOE Contact: N. L. Garland, 202-586-5673
ORNL Contact: T. R. Armstrong, 865-574-7996

The goal of this effort is to develop a metallic alloy capable of forming a defect-free, corrosion-resistant nitride surface layer during gas nitridation to enable use as a bipolar plate in PEM fuel cells. The nitrided alloy must be capable of meeting the DOE 10/kW bipolar plate target. Preliminary results indicate that alloying/process modification to a Fe-27Cr base alloy have succeeded in forming a dense, protective Cr-nitride layer, similar to that formed on Ni-Cr base alloys. This is a key development because the cost of this alloy is estimated to be 5-10 x less than the Ni-Cr base alloys studied/developed under this effort. This is the first time such a surface has been successfully formed on a Fe-Cr base alloy. (This is a more robust and corrosion-resistant surface than the nitrogen modified passive oxide layer effect previously demonstrated for commercially available ferritic alloys such as 446 and AL 29-4C). Thus far, cathode environment screening and as-nitrided interfacial contact resistance measurements show behavior equal to that of nitrided Ni-50Cr. Anode environment screening and a second round of optimization followed by fuel cell testing is planned. An invention disclosure is planned.

Coupons of nitrided commercial Ni-Cr alloys HASTELLOY G-30 and G-35 passed corrosion and contact resistance screenings in testing at General Motors (GM). Plates for single-cell fuel cell testing at GM will be manufactured and similar testing is also planned with Fuel Cell Energy. Test plates of nitrided Ni-50Cr, G-30, G-35, and AL 29-4C were manufactured and delivered to MTI Fuel Cells for single-cell testing, based on successful corrosion and contact resistance coupon results at MTI earlier. A 4 mil thick foil of G-35 stamped by GENCELL was successfully nitrided. Little warpage was observed, and although some technical challenges exist, no “show stopper” phenomena were observed in this first attempt.

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

86. COMPACT CARBON FOAM RADIATOR FOR FUEL CELL POWER SYSTEMS
$142,500
DOE Contact: N. L. Garland, 202-586-5673
ORNL Contact: T. R. Armstrong, 865-574-7996

The efficient operation of fuel-cell-powered vehicles requires systems capable of managing heat flow among exothermic components that produce heat while in use and therefore require cooling (e.g., air compressor, water recovery condenser, fuel cell stack), and endothermic components that require heat to be operational (e.g., water vaporizers). The outstanding thermal properties of graphite and its low density have prompted efforts to investigate the feasibility of using this material for the fabrication of thermal management system components, such as heat exchangers, condensers and vaporizers for fuel-cell-powered vehicles. Among the various forms of graphite, graphite fibers are ideal candidates for the fabrication of thermal management components because of their low density, high thermal conductivity, outstanding mechanical properties and commercial availability. Furthermore, graphite fibers can be woven to produce lightweight, robust, 3-D structures using standard textile technologies. The architecture of such woven fiber structures can be designed and optimized through experimental and modeling work. The type of fiber and their orientation in the woven structure can be selected to maximize heat transfer while minimizing cost. The geometrical features of the woven structure (e.g., weaving pattern) and their scale (e.g., spacing between fill and warp bundles) can be determined in order to minimize pressure drop.

Keywords: Carbon, Radiator, Heat Exchanger, Thermal Management

87. SELECTIVE CATALYTIC OXIDATION OF HYDROGEN SULFIDE
$350,000
DOE Contact: N. L. Garland, 202-586-5673
ORNL Contact: T. R. Armstrong, 865-574-7996

The objective of this work is to develop and optimize low-cost carbon-based catalysts for the selective oxidation process to reduce sulfur levels to the parts per billion range in a H_2-rich gas stream using low-cost carbon-based catalysts to produce a low to zero-sulfur fuel for use in fuel cells. In addition, in this project different activation protocols and carbon-based precursors that can lead to improved catalytic properties will be investigated, the microstructures, surface properties, and impurity level of the catalysts will be characterized and correlated to catalytic activity, selectivity, and durability.

Proof of principle has already been established and carbon catalysts developed by ORNL have been tested in several H_2-rich streams and demonstrated the capability of continuous removal of sulfur to less than 200 ppb levels. The undesired formation of gaseous sulfur by-products such as sulfur dioxide (SO_2) and carbonyl sulfide (COS) is a key aspect for the successful performance of the catalysts and one of the main challenges. Catalytic evaluation of the synthesized activated carbon and numerous commercial activated carbons based on wood, coal, cellulose, and coconut shells was in a fixed-bed reactor system. The selective oxidation reaction was conducted at temperatures in the range of 100-200^{o} C at atmospheric pressure with a space velocity of 3100 h^{-1}. Several reaction parameters were varied to investigate the reaction mechanism.

Keywords: Carbon Catalyst, Sulfur Removal, Fuel Processing

INDUSTRIAL TECHNOLOGIES PROGRAM

	FY 2004
INDUSTRIAL TECHNOLOGIES PROGRAM - GRAND TOTAL	$16,051,426
ALUMINUM SUBPROGRAM	$5,351,635
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,514,799
Reduction of Oxidative Melt Loss of Aluminum	400,000
Selective Adsorption of Salts from Molten Aluminum	68,566
Aluminum Carbothermic Technology	814,721
High Efficiency Low Dross Combustion System	52,986
Gas Fluxing of Aluminum	78,526
Microwave Assisted Electrolytic Cell	100,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$2,397,588
Reduction of Annealing Times for Energy Conservation in Aluminum Processing	81,479
Surface Behavior of Aluminum Alloys Deformed under Various Processing Conditions	85,124
Fundamental Studies of Structural Factors Affecting the Formability of Continuous Cast Aluminum Alloys	100,000
Development of a Two-phase Model for the Hot Deformation of Highly-Alloyed Aluminum	89,025
Development of Integrated Methodology for Thermo-mechanical Processing of Aluminum Alloys	114,697
Numerical Modeling of Transient Melt Flows and Interface Instability in Aluminum Reduction Cells	56,865
Low Temperature Reduction of Alumina Using Fluorine Containing Ionic Liquids	99,067
Effect of Impurities on the Processing of Aluminum Alloys in Casting, Extrusion, and Rolling	100,000
Combined Experimental and Computational Approach for the Design of Mold Surface Topography	100,000
Molten Aluminum Treatment by Salt Fluxing with Low Environmental Emissions	106,638
Inert Metal Anodes for Primary Aluminum Production	400,000
Improved Energy Efficiency in Aluminum Melting	971,898
Evaluation and Characterization of In-Line Annealed Continuous Cast Aluminum Sheet	92,795
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,439,248
Spray Rolling Aluminum Strip	250,000
Modeling Optimization of Direct Chill Casting	75,077
Degassing of Aluminum Alloys Using Ultrasonic Vibrations	60,000
Effect of Casting Conditions & Composition on Microstructural Gradients in Roll Cast Aluminum Alloys	90,326
Energy Efficient Isothermal Melting of Aluminum	718,021
Continuous Severe Deformation Processing of Aluminum Alloys	184,024
Development of a Rolling Process Design Tool for Use in Improving Hot Roll Slab Recovery	61,800
METAL CASTING SUBPROGRAM	$643,466
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$121,466
Development of Elevated Temperature Aluminum MMC Alloy	28,263
Development of Surface Engineered Coatings for Die Casting Dies	93,203

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2004
METAL CASTING SUBPROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING	$522,000
Aging of Graphitic Cast Irons and Machinability	45,000
Corrosion Testing Practices for High Alloys	46,000
Advanced Lost Foam Casting Technology	225,000
Development of CCT Diagrams for High Alloys Steels	36,000
Improved Die Casting Process to Preserve the Life of the Inserts	80,000
Characterization of Surface Anomalies from Magnetic Particle and Liquid Penetrant Indications	90,000
STEEL SUBPROGRAM	NA[1]
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$15,976,548
Controlled Thermo-Mechanical Processing of Tubes and Pipes for Enhanced Manufacturing and Performance	13,439,040
Life Improvement of Pot Hardware in Continuous Hot Dipping Processes	2,289,000
Plant Trial of Non-Chromium Passivation Systems for Electrolytic Tin Plate	248,508
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$10,621,507
Research Related to the Development of the Automated Steel Cleanliness Analysis Tool (ASCAT)	1,992,318
Enhanced Inclusion Removal from Steel in the Tundish	813,045
Reducing the Variability of HSLA Sheet Steels	548,168
Constitutive Behavior of High Strength Multiphase Sheet Steels under High Strain Rate Deformation	1,023,060
Clean Steel - Advancing the State of the Art	421,612
Characterization of Formability of Advanced High Strength Steels	1,007,959
Development of a Standard Methodology for Quantitative Measurement of Steel Phase Transformation Kinetics and Dilation Strains Using Dilatometric Methods	1,152,348
Characterization of Fatigue and Stress/Strain Behavior in Advanced High Strength Steels	385,221
Validation of Hot Strip Mill Model	2,594,476
Inclusion Optimization for New Generation Steel Products	448,210
Development of Appropriate Spot Welding Practice for Advanced High Strength Steels	235,090
MATERIALS PREPARATION, SYNTHESIS DEPOSITION, GROWTH OR FORMING	$6,377,008
Ironmaking Challenge - The Mesabi Nugget Research Project	5,555,008
Development of Steel Foam Materials and Structures	822,000

[1]For every project within the American Iron and Steel Institute's (AISI) Technology Roadmap Program (TRP), the funding shown is the budgeted total over the life of the project. Total DOE/ITP TRP funding to date (up to FY05) is $20,541,238. Separate FY04 funding data are not available.

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2004
MATERIALS SUBPROGRAM	$10,056,325
DEGRADATION RESISTANT MATERIALS	$6,293,525
MATERIALS DEVELOPMENT AND PROCESSING	$1,660,334
Development of Stronger and More Reliable Cast Austenitic Stainless Steels (H-Series) Based on Scientific Design Methodology	80,000
High Density Infrared (HDI) Transient Liquid Coatings (TLC) for Improved Wear and Corrosion Resistance	299,116
Low-Temperature Surface Carburizing of Stainless Steels	419,250
Fracture Toughness and Strength in a New Class of Bainitic Chromium-Tungsten Steels	92,894
Development of a New Class of Fe-3Cr-W (V) Ferritic Steels for Industrial Process Applications	475,000
Physical and Numerical Analysis of Extrusion Process for Production of Bi-Metallic Tubes	169,074
Ultrasonic Processing of Materials	125,000
ULTRA–HARD MATERIALS	$660,000
Development of Bulk Nanocrystalline Cemented WC for Industrial Applications	290,000
Crosscutting Industrial Applications of a New Class of Ultra-Hard Borides	370,000
Development of Ultrananocrystalline Diamond (UNCD) Coatings for SiC Multipurpose Mechanical Pump Seals	1,000,000
WEAR/CORROSION RESISTANT MATERIALS	$2,973,191
Advanced Composite Coatings for Industries of the Future	150,000
Advanced Wear and Corrosion Resistant Systems Through Laser Surface Alloying	120,000
Alkaline-Resistant Fe-Phosphate Glass Fibers as Concrete Reinforcement	240,000
Development of Functionally Graded Materials for Manufacturing Tools	581,250
Development of Materials Resistant to Metal Dusting	337,000
Novel Carbon Films for Next Generation Rotating Equipment Applications	100,000
High-Performance, Oxide-Dispersion-Strengthened Tubes for Production of Ethylene and Other Industrial Chemicals	211,044
Stress-Assisted Corrosion in Boiler Tubes	753,897
Structurally Integrated Coatings for Wear and Corrosion	480,000
THERMOPHYSICAL DATABASES AND MODELING	$954,000
Development of Combinatorial Methods for Alloy Design and Optimization	160,000
Inverse Process Analysis for the Acquisition of Thermophysical Property Data	215,000
Prediction of Corrosion of Advanced Materials and Fabricated Components	579,000
MATERIALS FOR SEPARATIONS	$181,000
Novel Modified Zeolites for Energy-Efficient Hydrocarbon Separations	181,000

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2004
MATERIALS SUBPROGRAM (continued)	
MATERIALS FOR ENERGY SYSTEMS	$2,627,800
REFRACTORIES/HEAT RECOVERY	$2,061,000
Advanced Thermoelectric Materials for Effective Waste Heat Recovery in Process Industries	625,000
High Density Infrared Treatment of Refractories	138,000
Materials for High-Temperature Black Liquor Gasification	100,000
Multifunctional Metallic and Refractory Materials for Handling of Molten Metals	668,000
Materials for Industrial Heat Recovery Systems	530,000
WELDING/JOINING	$566,800
Advanced Integration of Multi-Scale Mechanics and Welding Process Simulation in Weld Assessment	400,000
Virtual Welded-Joint Design Integrating Advanced Materials and Processing Technologies	166,800

INDUSTRIAL TECHNOLOGIES PROGRAM

ALUMINUM SUBPROGRAM

The DOE Aluminum Team leader is Charles Sorrell (202) 586-1514

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

88. REDUCTION OF OXIDATIVE MELT LOSS OF ALUMINUM
$400,000
DOE Contact: Charles Sorrell, 202-586-1514

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

89. SELECTIVE ADSORPTION OF SALTS FROM MOLTEN ALUMINUM
$68,566
DOE Contact: Charles Sorrell, 202-586-1514

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

90. ALUMINUM CARBOTHERMIC TECHNOLOGY
$814,721
DOE Contact: Charles Sorrell, 202-586-1514

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 power consumption in the range of 9.5 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

91. HIGH EFFICIENCY LOW DROSS COMBUSTION SYSTEM
    $52,986
    DOE Contact: Charles Sorrell, 202-586-1514

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

92. GAS FLUXING OF ALUMINUM
    $78,526
    DOE Contact: Charles Sorrell, 202-586-1514

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

93. MICROWAVE ASSISTED ELECTROLYTIC CELL
    $100,000
    DOE Contact: Charles Sorrell, 202-586-1514

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

94. REDUCTION OF ANNEALING TIMES FOR ENERGY CONSERVATION IN ALUMINUM PROCESSING
    $81,479
    DOE Contact: Charles Sorrell, 202-586-1514

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

95. SURFACE BEHAVIOR OF ALUMINUM ALLOYS DEFORMED UNDER VARIOUS PROCESSING CONDITIONS
    $85,124
    DOE Contact: Charles Sorrell, 202-586-1514

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

96. FUNDAMENTAL STUDIES OF STRUCTURAL FACTORS AFFECTING THE FORMABILITY OF CONTINUOUS CAST ALUMINUM ALLOYS
    $100,000
    DOE Contact: Charles Sorrell, 202-586-1514

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

97. DEVELOPMENT OF A TWO-PHASE MODEL FOR THE HOT DEFORMATION OF HIGHLY-ALLOYED ALUMINUM
    $89,025
    DOE Contact: Charles Sorrell, 202-586-1514

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

98. DEVELOPMENT OF INTEGRATED METHODOLOGY FOR THERMO-MECHANICAL PROCESSING OF ALUMINUM ALLOYS
$114,697
DOE Contact: Charles Sorrell, 202-586-1514

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

99. NUMERICAL MODELING OF TRANSIENT MELT FLOWS AND INTERFACE INSTABILITY IN ALUMINUM REDUCTION CELLS
$56,865
DOE Contact: Charles Sorrell, 202-586-1514

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

100. LOW-TEMPERATURE REDUCTION OF ALUMINA USING FLUORINE CONTAINING IONIC LIQUIDS
$99,067
DOE Contact: Charles Sorrell, 202-586-1514

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

101. EFFECT OF IMPURITIES ON THE PROCESSING OF ALUMINUM ALLOYS
$100,000
DOE Contact: Charles Sorrell, 202-586-1514

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

102. COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACH FOR THE DESIGN OF MOLD SURFACE TOPOGRAPHY
$100,000
DOE Contact: Charles Sorrell, 202-586-1514

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

103. MOLTEN ALUMINUM TREATMENT BY SALT FLUXING WITH LOW ENVIRONMENTAL EMISSIONS
$106,638
DOE Contact: Charles Sorrell, 202-586-1514

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

104. INERT METAL ANODES FOR PRIMARY ALUMINUM PRODUCTION
$400,000
DOE Contact: Charles Sorrell, 202-586-1514

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

105. IMPROVED ENERGY EFFICIENCY IN ALUMINUM MELTING
$971,898
DOE Contact: Charles Sorrell, 202-586-1514

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

106. EVALUATION AND CHARACTERIZATION OF IN-LINE ANNEALED CONTINIOUS CAST ALUMINUM SHEET
$92,795
DOE Contact: Charles Sorrell, 202-586-1514

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

107. SPRAY ROLLING ALUMINUM STRIP
$250,000
DOE Contact: Charles Sorrell, 202-586-1514
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

108. MODELING OPTIMIZATION OF DIRECT CHILL CASTING
$75,077
DOE Contact: Charles Sorrell, 202-586-1514

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

109. DEGASSING OF ALUMINUM ALLOYS USING ULTRASONIC VIBRATIONS
$60,000
DOE Contact: Charles Sorrell, 202-586-1514

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

110. EFFECT OF CASTING CONDITIONS AND COMPOSITION ON MICROSTRUCTURAL GRADIENTS IN ROLL CAST ALUMINUM ALLOYS
$90,326
DOE Contact: Charles Sorrell, 202-586-1514

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

111. ENERGY EFFICIENT ISOTHERMAL MELTING OF ALUMINUM
$718,021
DOE Contact: Charles Sorrell, 202-586-1514

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

112. CONTINUOUS SEVERE PLASTIC DEFORMATION PROCESSING OF ALUMINUM ALLOYS
$184,024
DOE Contact: Charles Sorrell, 202-586-1514

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

113. DEVELOPMENT OF A ROLLING PROCESS DESIGN TOOL FOR USE IN IMPROVING HOT ROLL SLAB YIELD
$61,800
DOE Contact: Charles Sorrell, 202-586-1514

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

METAL CASTING SUBPROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

114. DEVELOPMENT OF ELEVATED TEMPERATURE ALUMINUM MMC ALLOY
$28,263
DOE Contact: Ehr Ping HuangFu, 202-586-1493
Eck Industries, Inc., Contact: Dave Weiss, 920-682-4618

The objectives of this project are to: select a ceramic or intermetallic reinforcement that is chemically stable at elevated temperature in an aluminum matrix that does not contain silicon; devise a low-cost, liquid-metal mixing technology that can homogeneously incorporate fine (5 to 8 micron diameter) particulates into an aluminum alloy itself having good elevated temperature mechanical properties; select alloy chemistries that provide solid solution strengthening of the primary matrix and have good fracture toughness properties; and assure that the resultant alloy system may be cast into high quality components using cost effective production methods. The expected mechanical properties will also be verified.

Keywords: Aluminum, MMC, Alloy

115. DEVELOPMENT OF SURFACE ENGINEERED COATINGS FOR DIE CASTING DIES
$93,203
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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

116. AGING OF GRAPHITIC CAST IRONS AND MACHINABILITY
$45,000
DOE Contact: Ehr Ping HuangFu, 202-586-1493
University of Missouri, Rolla Contact: Von Richard, 573-341-4730

The goals of this project are to: determine whether ductile iron and compacted graphite iron exhibit age strengthening to a statistically significant extent; identify the mechanism by which gray iron age strengthens ; ientify the mechanism by which age-strengthening improves the machinability of gray cast iron; dtermine whether age strengthening improves the machinability of ductile iron and compacted graphite iron alloys; dvelop a predictive model of alloy factor effects on age strengthening .

Keywords: Metal Casting, Aging, Graphitic Cast Iron, Machinability

117. CORROSION TESTING PRACTICES FOR HIGH ALLOYS
$46,000
DOE Contact: Ehr Ping HuangFu, 202-586-1493
Lehigh University Contact: John N. DuPont, 610-758-3942

The objectives of this research project are to: determine the influence of ASTM crevice, pitting, and intergranular corrosion test variables on reproducibility of results; suggest changes to the ASTM corrosion methods that will permit accurate use of these test procedures as a material acceptance standard; and determine the influence of thermal conditions (including changes in Niyama values) on the microsegregation potential and concomitant corrosion resistance of high alloy castings.

Keywords: Metal Casting, High Alloys, Corrosion Tests

118. ADVANCED LOST FOAM CASTING TECHNOLOGY
$225,000
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: Metal Casting, Lost Foam Casting

119. DEVELOPMENT OF CCT DIAGRAMS FOR HIGH ALLOY STEELS
$36,000
DOE Contact: Ehr Ping HuangFu, 202-586-1493
Iowa State University Contact: L. Scott Chumbley, 515-294 7903

This research project seeks to use detailed metallographic examinations, possibly supplemented by dilatometry measurement techniques, to determine the phase transformation processes and the kinetics of those processes in state-of-the-art, high-Mo superaustenitic stainless steel casting alloys. The alloys of interest are CK3MCuN and CN-3MN. Transformation kinetics will be determined for both isothermal and continuously cooling conditions to yield TTT and CCT diagrams, respectively. Metallographic examinations will involve extensive image analysis using optical microscopy and secondary and transmission electron microscopies. Interpretation of the transformation behaviors observed will be aided using the thermodynamic software package *Thermo-Calc*. The results generated from this program will be invaluable for both understanding and controlling the role of the various phase transformations during the production of castings of different section thickness.

Keywords: Metal Casting, Transformation Diagram, High Alloys

120. IMPROVED DIE CASTING PROCESS TO PRESERVE THE LIFE OF THE INSERTS
$80,000
DOE Contact: Ehr Ping HuangFu, 202-586-1493
Case Western Reserve University Contact: Jack Wallace, 216) 368-4222

The goal of this project is to study the combined effects of die design, proper internal cooling and efficient die lubricants on die life and develop methods of optimized process control for extended die life. The combination of die design, proper internal cooling and the efficient utilization of die lubricants will provide much longer die life. Data developed in this project will be of great value to the die casting industry in developing die life extension methods. The impact of these methods on energy consumption is very significant. By proper internal water cooling, a more stable, higher die temperature can be maintained thus not only extending die life but also preserving energy by using lower pouring temperatures.

Keywords: Metal Casting, Die Casting, Die Life, Inserts

121. CHARACTERIZATION OF SURFACE ANOMALIES FROM MAGNETIC PARTICLES AND LIQUID PENETRANT INDICATIONS
$90,000
DOE Contact: Ehr Ping HuangFu, 202-586-1493
University of Alabama, Birmingham Contact: Charles Bates, 205) 975-8120

The objective of this research project are to: characterize surface/near surface indications and develop an inspection and analysis protocol; collect a variety of surface/near indications from participating foundries with the appropriate ASTM rating as measured by the foundry; metallurgically characterize each anomaly to determine source, size, shape, depth, and sharpness.

Keywords: Metal Casting, Characterization, Surface Anormaly, Magnetic Particles

STEEL SUBPROGRAM[1]

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

122. CONTROLLED THERMO-MECHANICAL PROCESSING OF TUBES AND PIPES FOR ENHANCED MANUFACTURING AND PERFORMANCE
$13,439,040
DOE Contact: Simon Friedrich, 202-586-6759 and Debo Aichbhaumik, 303-275-4763
The Timken Company Contact: Robert Kolarik, 330-471-2378

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

Keywords: Thermomechanical Processing, Modeling, Microstructure

123. LIFE IMPROVEMENT OF POT HARDWARE IN CONTINUOUS HOT DIPPING PROCESSES
$2,289,000
DOE Contact: Simon Friedrich, 202-586-6759 and Debo Aichbhaumik, 303-275-4763
West Virginia University Contact: Keh-Minn Chang

The objectives of this project are to develop new bulk materials and surface treatment/coatings for life improvement of molten metal bath hardware and

[1]For every project within the American Iron and Steel Institute's (AISI's) Technology Roadmap Program (TRP), the funding shown is the budgeted total over the life of the project. Total DOE/ITP TRP funding to date (up to FY05) is $20,541,238. Separate FY04 funding data are not available.

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

Keywords: Pot Hardware, Hot Dip Processing, Lifetime

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

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

Keywords: Electrolytic Tin Plate, Passivation, Chromium-Free

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

125. RESEARCH RELATED TO THE DEVELOPMENT OF THE AUTOMATED STEEL CLEANLINESS ANALYSIS TOOL (ASCAT)
$1,992,318
DOE Contact: Simon Friedrich, 202-586-6759 and Debo Aichbhaumik, 303-275-4763
RJ Lee Group Contact: Gary Casuccio, 724-387-1818

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

Keywords: Steel, Automation, Cleanliness Analysis

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

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

Keywords: Computational Fluid Dynamics, Modeling, Inclusion Removal

127. REDUCING THE VARIABILITY OF HSLA SHEET STEELS
$548,168
DOE Contact: Simon Friedrich, 202-586-6759 and Debo Aichbhaumik, 303-275-4763
University of Pittsburgh Contact: Anthony DeArdo, deardo@engrng.pitt.edu
AISI Contact: Joe Vehec, 412-922-2772

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

Keywords: High-Strength Steels, Variability

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

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

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

129. CLEAN STEEL - ADVANCING THE STATE OF THE ART
$421,612
DOE Contact: Simon Friedrich, 202-586-6759
and Debo Aichbhaumik, 303-275-4763
Carnegie Mellon University Contact:
Alan W. Cramb, 412-268-5548
AISI Contact: Joe Vehec, 412-922-2772

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

Keywords: Steel, Inclusion Removal

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

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

Keywords: High-Strength Steels, Formability

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

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

Keywords: Steel, Transformation, Dilatometer, Gleeble

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

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

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

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

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

Keywords: Steel, Hot Strip Mill, Modeling

134. INCLUSION OPTIMIZATION FOR NEW GENERATION STEEL PRODUCTS
$448,210
DOE Contact: Simon Friedrich, 202-586-6759 and Debo Aichbhaumik, 303-275-4763
Carnegie Mellon University Contact: Alan W. Cramb, 412-268-5548
AISI Contract: Joe Vehec, 412-922-2772

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

Keywords: Steel, Inclusion Optimization

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

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

Keywords: High-Strength Steels, Spot Welding

MATERIALS PREPARATION, SYNTHESIS DEPOSITION, GROWTH OR FORMING

136. IRONMAKING CHALLENGE - THE MESABI NUGGET RESEARCH PROJECT
$5,555,008
DOE Contact: Simon Friedrich, 202-586-6759 and Debo Aichbhaumik, 303-275-4763
Mesabi Nugget, LLC Contact: Larry Lehtinen, 218-226-6206

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

Keywords: Ironmaking, Rotary Hearth, Mesabi Nugget Project

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

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

Keywords: Steel, Foam, Powder Metallurgy

MATERIALS SUBPROGRAM

New or improved materials can save significant energy and improve productivity by enabling systems to operate at higher temperatures, last longer, and reduce capital costs. The Materials subprogram is a crosscutting program with emphasis on meeting the industrial needs of energy-intensive processing industries. Efforts in FY 2004 were focused on the research, design, development, and testing of new and improved materials, as well as more profitable uses of existing materials, for energy efficient industrial processes. The projects are grouped in the following categories 1) Degradation Resistant Materials, 2) Databases and Modeling, 3) Materials for Separations, and (4) Materials for Energy Systems and project descriptions are included below. The DOE program manager is Sara Dillich (202) 586-7925.

DEGRADATION RESISTANT MATERIALS

MATERIALS DEVELOPMENT AND PROCESSING

138. DEVELOPMENT OF STRONGER AND MORE RELIABLE CAST AUSTENITIC STAINLESS STEELS (H-SERIES) BASED ON SCIENTIFIC DESIGN METHODOLOGY
$80,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

139. HIGH DENSITY INFRARED (HDI) TRANSIENT LIQUID COATINGS (TIC) FOR IMPROVED WEAR AND CORROSION RESISTANCE
$299,116
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

140. LOW-TEMPERATURE SURFACE CARBURIZING OF STAINLESS STEELS
$419,250
DOE Contact: Sara Dillich, 202-586-7925

The objective of this research is to develop and evaluate a new processing method, low temperature colossal supersaturation (LTCSS), for improving the surface hardness and degradation resistance of austenitic stainless steels. A novel surface carburization treatment for 316 austenitic stainless steels that produces a colossal supersaturation of carbon interstitials and a consequent increase of the surface hardness by a factor of four to five, along with improved corrosion- and wear-resistance, has recently been developed . This novel approach can be applied to other stainless steel compositions with further improvements in properties. To realize the full potential of this technology, the research team will process a suite of commercial austenitic stainless steels; the team members will analyze the LTCSS process, characterize the carburized parts, and evaluate the improvement in energy efficiency offered by LTCSS of austenitic stainless steels. The research will allow substantial reduction of the service-induced wear of austenitic stainless steel parts in a variety of applications, including, for example, impeller pumps for the chemical and petroleum industries.

Keywords: Low-Temperature, Stainless Steels, Surface Carburization, Supersaturation, Surface Hardness, Degradation Resistance

141. FRACTURE TOUGHNESS AND STRENGTH IN A NEW CLASS OF BAINITIC CHROMIUM-TUNGSTEN STEELS
$92,894
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

142. DEVELOPMENT OF A NEW CLASS OF FE-3CR-W (V) FERRITIC STEELS FOR INDUSTRIAL PROCESS APPLICATIONS
$475,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

143. PHYSICAL AND NUMERICAL ANALYSIS OF EXTRUSION PROCESS FOR PRODUCTION OF BI-METALLIC TUBES
$169,074
DOE Contact: Sara Dillich, 202-586-7925

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

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

144. ULTRASONIC PROCESSING OF MATERIALS
$125,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

ULTRA–HARD MATERIALS

145. DEVELOPMENT OF BULK NANOCRYSTALLINE CEMENTED WC FOR INDUSTRIAL APPLICATIONS
$290,000
DOE Contact: Sara Dillich, 202-586-7925

The overall project goals are to develop bulk nanocrystalline WC-Co cermet materials for a wide variety of industrial applications and to enable the commercialization of the process for manufacturing these materials. Scope of the project involves development of an economically viable process for making nanocrystalline WC/Co powder based on vapor phase synthesis., development of the ultrahigh pressure rapid heating and consolidation process to achieve < 100nm grain sizes, in depth study of mechanical properties of nanocrystalline WC-Co, establishment of an infrastructure for the commercialization of the production technology developed under this project, and proof of concept field tests. Successful completion of the proposed project will offer some of the first nano materials for industrial applications

Keywords: Bulk Nanocrystalline, Nanocrystalline, Cermet, Vapor Phase Synthesis, Ultrahigh Pressure Rapid Heating

146. CROSSCUTTING INDUSTRIAL APPLICATIONS OF A NEW CLASS OF ULTRA-HARD BORIDES
$370,000
DOE Contact: Sara Dillich, 202-586-7925
Ames Laboratory, Iowa State University Contact: Bruce Cook, 515-294-9673

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

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

147. DEVELOPMENT OF ULTRANANOCRYSTALLINE DIAMOND (UNCD) COATINGS FOR SiC MULTIPURPOSE MECHANICAL PUMP SEALS
$1,000,000
DOE Contact: Sara Dillich, 202-586-7925
ANL Contact: John Hryn, 630-252-5894

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

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

WEAR/CORROSION RESISTANT MATERIALS

148. ADVANCED COMPOSITE COATINGS FOR INDUSTRIES OF THE FUTURE
$150,000
DOE Contact: Sara Dillich, 202-586-7925
PNNL Contact: Charles Henager, Jr., 509-376-1442

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

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

149. ADVANCED WEAR AND CORROSION RESISTANT SYSTEMS THROUGH LASER SURFACE ALLOYING
$120,000
DOE Contact: Sara Dillich, 202-586-7925
Applied Research Laboratory, Pennsylvania State University Contact: R. P. Martukanitz, rxm44@psu.edu

The objective of this research is to use laser processing techniques to develop and implement ultra-hard coatings through the formation of wear resistant, composite surface structures. During the first year, emphasis will be placed on the refinement, integration, and verification of process and materials simulation techniques capable of developing composite coating systems and processing that provide superior performance characteristics. Continued theoretical evaluation of new material components and processing conditions will be utilized in conjunction with laboratory trials during this period. The second year will include full implementation of the advanced coating technology through verifications and demonstrations directed at specific industry applications. During this period, test to determine improvements in performance and economic analysis will also be used to quantify the benefits associated with the advanced laser-based coating systems developed under this project.

Keywords: Advanced Wear, Corrosion Resistant, Laser Surface Alloying, Materials Simulation, Composite Coating Systems

150. ALKALINE-RESISTANT Fe-PHOSPHATE GLASS FIBERS AS CONCRETE REINFORCEMENT
$240,000
DOE Contact: Sara Dillich, 202-586-7925

The objective is to perform advanced research to evaluate selected Fe-phosphate glass fiber compositions for use in concrete reinforcement, and as an alternative to current silica-based fibers. Glass fibers compositions will be prepared using conventional melting procedure. Glass formation and important glass properties will be characterized using differential thermal analysis, Mossbauer, and Raman spectroscopy, to provide information on glass formation and structure. Complementary analysis such as microstructural and physical analyses of glass fibers and computer simulation of corrosion will also be conducted. Properties important to the performance of the glass fibers as effective concrete reinforcement, including chemical durability and strength, will also be measured. Tests recommended for concrete composites will be used for evaluation of resulting compositions.

Keywords: Fe-Phosphate, Glass Fibers, Concrete Reinforcement, Alkaline-Resistant

151. DEVELOPMENT OF FUNCTIONALLY GRADED MATERIALS FOR MANUFACTURING TOOLS
$581,250
DOE Contact: Sara Dillich, 202-586-7925

The objective of this research is to develop functionally graded structures made from ferrous- or nickel- based materials and composites, as well as unique near-net-shape manufacturing processes, Laser Powder Deposition (LPD) and solid state dynamic powder forging, to produce tools, dies and equipment for multiple manufacturing industries. Both graded metallic and graded metal-ceramic composites will be investigated in this project. These tools and dies are expected to provide significant reductions in energy consumption for various industrial processes through reduction of scrap and improved thermal management during manufacturing.

Keywords: Functionally Graded, Manufacturing Tools, Scrap Reduction, Thermal Management, Tools, Dies

152. DEVELOPMENT OF MATERIALS RESISTANT TO METAL DUSTING
$337,000
DOE Contact: Sara Dillich, 202-586-7925
Materials Technology Institute Contact:
Emory Ford, eaford@comcast.net

The objective of this research is to develop metallic alloys and surface engineering for commercial alloys to improve corrosion resistance and high temperature mechanical properties in order to mitigate metal dusting degradation during high temperature manufacturing processes. The alloys will have an improved corrosion resistance and will also possess adequate mechanical properties at temperatures up to 1500˚F. The project will involve design and construction of a high-pressure test facility (with capability for exposure of multiple specimens) for the exposure of candidate alloys and surface-engineered alloys to metal dusting environments that simulate the temperatures, pressures, and chemistry prevalent in hydrogen and ammonia reformers and in syngas systems. The project will also develop a database on metal dusting degradation from the standpoint of incubation time, general corrosion, pitting attack, pitting rate and size for the candidate alloys as a function of the process variables.

Keywords: Metal Dusting, High Temperature, Corrosion Resistance, Degradation

153. NOVEL CARBON FILMS FOR NEXT GENERATION ROTATING EQUIPMENT APPLICATIONS
$100,000
DOE Contact: Sara Dillich, 202-586-7925

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

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

154. HIGH-PERFORMANCE, OXIDE-DISPERSION-STRENGTHENED TUBES FOR PRODUCTION OF ETHYLENE AND OTHER INDUSTRIAL CHEMICALS
$211,044
DOE Contact: Sara Dillich, 202-586-7925

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

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

155. STRESS-ASSISTED CORROSION IN BOILER TUBES
$753,897
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

156. STRUCTURALLY INTEGRATED COATINGS FOR WEAR AND CORROSION
$480,000
DOE Contact: Sara Dillich, 202-586-7925

The objective of this research is to develop cost effective materials and processing solutions for wear and corrosion resistance of engineering components. Processes to be investigated include cladding via high intensity arc lamp processing, hybrid laser assisted thermal spray, hybrid laser arc welding, and plasma transferred arc welding. Modeling will be used to aid in the materials and process development by providing insight into the materials microstructures resulting from the candidate processes.

Keywords: Wear, Corrosion, Coatings

THERMOPHYSICAL DATABASES AND MODELING

157. DEVELOPMENT OF COMBINATORIAL METHODS FOR ALLOY DESIGN AND OPTIMIZATION
$160,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

Keywords: Combinatorial, Alloy Design, Carburization, Corrosion

158. INVERSE PROCESS ANALYSIS FOR THE ACQUISITION OF THERMOPHYSICAL PROPERTY DATA
$215,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

Keywords: Dilatometry, Thermophysical Properties, Differential Scanning Calorimetry

159. PREDICTION OF CORROSION OF ADVANCED MATERIALS AND FABRICATED COMPONENTS
$579,000
DOE Contact: Sara Dillich, 202-596-7925

This project will combine fundamental understanding of mechanisms of corrosion with focused experimental results to predict the corrosion of advanced fabricated alloys in operating environments encountered in the chemical and other processing industries. The focus of the project is to develop a generalized methodology and a tool to predict the performance of fabricated materials in corrosive environments. The goal is to develop a tool that will predict corrosion performance of fabricated components in any environment utilizing a minimum data set. The objectives of the project will include selection of alloys, treatment methods, and representative process environments; development of an experimental database of alloy microchemistry in relation to fabrication process and electrochemical parameters; extension of models and methodology for prediction of localized corrosion; and encapsulation of the models in engineering software.

Keywords: Corrosion, Advanced Fabricated Alloys, Prediction Tool, Fabricated Materials

MATERIALS FOR SEPARATIONS

160. NOVEL MODIFIED ZEOLITES FOR ENERGY-EFFICIENT HYDROCARBON SEPARATIONS
$181,000
DOE Contact: Sara Dillich, 202-586-7925
Sandia National Laboratories contact: T. M. Nenoff 505-844-0340

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

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

MATERIALS FOR ENERGY SYSTEMS

REFRACTORIES/HEAT RECOVERY

161. ADVANCED THERMOELECTRIC MATERIALS FOR EFFECTIVE WASTE HEAT RECOVERY IN PROCESS INDUSTRIES
$625,000
DOE Contact: Sara Dillich, 202-586-7925

The objective of this research is to develop high efficiency thermoelectric energy conversion materials and technology to recover waste energy from exhaust gas and other infrastructure heat losses in industrial processing plants. The project will investigate, develop and deploy high efficiency thermoelectric (TE) energy conversion technology to recover waste energy from exhaust gas in glass manufacturing plants. New technology in thermoelectric materials will be combined with advanced capabilities in modeling to design and develop thermoelectric generators that can be used in glass production facilities and other waste heat stacks. The electrical power recovered from waste heat can be used in glass production or returned to the electrical grid.

The project will involve the development of thin film thermoelectric materials, fabrication of prototype generators, bench testing of generators in configurations simulating conditions encountered in the glass industry, modeling of heat transfer processes to provide guidance for system integration, design of prototype thermoelectric generators for implementation in waste heat stacks, and finally, preliminary economic analyses for implementing this technology.

Keywords: Thermoelectric, Waste Heat, Heat Losses, Thin Film, Generators

162. HIGH DENSITY INFRARED TREATMENT OF REFRACTORIES
$138,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

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

163. MATERIALS FOR HIGH-TEMPERATURE BLACK LIQUOR GASIFICATION
$100,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: James Keiser, keiserj@ornl.gov

The industrial viability of high temperature, atmospheric pressure gasification technology depends on optimal integrity of structural components including refractories, and other materials, and on increasing the throughput capacity of processing black liquor by approximately 50%. The goal of this effort is to develop and evaluate improved corrosion resistant refractories and other structural components for use in high-throughput gasification.

Keywords: High-Temperature, Black Liquor, Gasification, Refractories

164. MULTIFUNCTIONAL METALLIC AND REFRACTORY MATERIALS FOR HANDLING OF MOLTEN METALS
$668,000
DOE Contact Sara Dillich, 202-586-7925

The objective of this research is to develop multifunctional materials and surface treatments to extend the life of containers and submerged hardware for molten metal production. Concern about liquid metal corrosion on containment and submerged hardware is a critical issue in metals processing industries. Heat loss due to degradation of refractories by corrosion and poor thermal management contributes further to energy inefficiencies. The research objectives of this project are to develop multifunctional metallic and refractory materials and surface treatment, coatings and claddings for life improvement of molten metal containment and submerged hardware and improved thermal management in aluminum, steel and metal casting industries.

Keywords: Multifunctional, Containers, Submerged Hardware, Molten Metal, Liquid Metal Corrosion, Coatings, Claddings

165. MATERIALS FOR INDUSTRIAL HEAT RECOVERY SYSTEMS
$530,000
DOE Contact: Sara Dillich, 202-586-7925

The objective of this research is to address materials solutions for enhanced heat recovery and reliability in Forest Products and Aluminum industrial systems. The project will concentrate on the recuperators associated with aluminum melting furnaces and the superheaters and wall tubes in black liquor recovery boilers. Failure modes for these componens, such as high temperature oxidation, intermediate temperature sulfidation, stress corrosion cracking and corrosion fatigue, will be investigated and materials for improved performance will be developed.

Keywords: Heat Recovery, Recuperators, Superheaters, Wall Tubes

WELDING/JOINING

166. ADVANCED INTEGRATION OF MULTI-SCALE MECHANICS AND WELDING PROCESS SIMULATION IN WELD ASSESSMENT
$400,000
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini

The objective of this research is to develop advanced methodology for assessment of weld performance and reliability for the chemical, energy, welding, and other manufacturing industries where performance of welds is a significant safety and economic factor. This research program will develop advanced methodology for weld performance and reliability assessment pertaining to the petroleum, chemical, energy, welding and other industry sectors where the performance of welds is a significant safety and economic factor. By integrating the disciplines of welding, materials science, micromechanics, fracture mechanics, and damage mechanics, this newly developed assessment procedures will lay the foundation to solve a number of challenging practical industry problems. The development will provide effective means for welding process optimization for structural reliability and performance that will increase the welding productivity and reduce the cost and energy associated with welding fabrication.

Keywords: Welding, Process Simulation, Fabrication, Multi-Scale Mechanics

167. VIRTUAL WELDED-JOINT DESIGN INTEGRATING ADVANCED MATERIALS AND PROCESSING TECHNOLOGIES
$166,800
DOE Contact: Sara Dillich, 202-586-7925
ORNL Contact: Peter Angelini, 865-576-8069

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

Keywords: Welding, Advanced Materials, Modeling, Fatigue

SOLAR ENERGY TECHNOLOGY PROGRAM

	FY 2004
SOLAR ENERGY TECHNOLOGY PROGRAM - GRAND TOTAL	$25,156,000
NATIONAL PHOTOVOLTAICS PROGRAM	$25,156,000
PHOTOVOLTAICS RESEARCH & DEVELOPMENT	$25,156,000
PHOTOVOLTAICS SUBPROGRAM OF THE SOLAR ENERGY TECHNOLOGIES PROGRAM (SETP)	$25,156,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$13,166,000
Thin-Film Amorphous Silicon, Thin-Film Polycrystalline Materials, and Silicon Film for Solar Cells	10,341,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	1,450,000
Nanocrystalline and Organic Solar Cell Materials	1,375,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,730,000
Materials And Device Characterization	6,780,000
Materials Structure And Composition	1,950,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$3,260,000
Materials Improvement For High-Efficiency Crystalline Silicon Solar Cells	2,360,000
Instrumentation and Facilities	900,000

SOLAR ENERGY TECHNOLOGY PROGRAM

OFFICE OF SOLAR ENERGY TECHNOLOGIES

NATIONAL PHOTOVOLTAICS PROGRAM

The Photovoltaics Subprogram of the Solar Energy Technologies Program (SETP) sponsors research and development with the goal of making terrestrial solar photovoltaic power a significant and commercially viable part of the national energy mix. Achievement of this goal implies installed photovoltaic systems with 30-year reliability and levelized lifetime user energy costs (2004 dollars) of approximately $0.06 / kWh. From such efforts, private enterprise can choose options for further development and competitive application in U.S. and foreign electric power markets. Manufacturing cost is affected by the expense of semiconductor materials growth and characterization, the complexity of junction formation and cell fabrication, and the material requirements of 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 2004 was 1194 MW, with 139 MW made in the United States.

The objective of materials research is to overcome technical barriers that limit the conversion efficiency, long-term reliability, and subsequent lifetime user energy cost of photovoltaic systems. Conversion efficiency of photovoltaic cells is limited by the spectral response of the semiconductor (dependent on band structure), inability to effectively collect energetic photogenerated carriers (hot carriers), carrier mobility in the material, and device engineering factors. Spectral response is limited by non-absorption of sub-bandgap photons. Additionally, energetic photons tend to be ineffectively used due to thermalization of “hot” carriers. Carrier mobility is dependent on material defects. Engineering 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 the dark recombination current (of excess photogenerated carriers). The Photovoltaics Subprogram of SETP includes subcontracts to develop so-called “Third Generation” photovoltaic material technologies which specifically address the efficiency limiting mechanisms of non-absorption of sub-bandgap photons and the thermalization of hot carriers. The SETP effort is also concerned with advanced materials that enhance module reliability.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

168. THIN-FILM AMORPHOUS SILICON, THIN-FILM POLYCRYSTALLINE MATERIALS, AND SILICON FILM FOR SOLAR CELLS
$10,341,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contacts: Ken Zweibel, 303-384-6441,
Bolko von Roedern, 303-384-6480,
Harin Ullal, 303-384-6486

The long term goal for amorphous silicon and polycrystalline thin films is to develop technologies for 15 percent efficient (stabilized) photovoltaic modules with cost under $50/m^2 and with 30-year lifetime. This will allow system lifetime user energy cost of approximately $0.06/kWh, and subsequent wide competition of thin-film photovoltaics for large-scale distributed power generation. (The goal for silicon film is to develop very high throughput crystalline silicon modules, with conversion efficiencies approximately 12-14 percent.)

Thin-Film Amorphous Silicon: These projects perform research on the deposition and characterization of amorphous silicon thin films to improve solar cell conversion efficiency and high-throughput manufacturability. Efficient conversion is hindered by the well-known, but still unresolved, light degradation effect characteristic of amorphous silicon PV devices, i.e., Staebler-Wronski Effect. The films are deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition and sputtering.

Thin-Film Polycrystalline Materials: These projects perform applied research on the deposition of CuIn(Ga,S)Se_2 (CIGSS) and CdTe polycrystalline thin films for solar cells. Research is focused on improving conversion efficiency by depositing more nearly stoichiometric CIGSS and CdTe films, by controlling interlayer diffusion and lattice matching in heterojunction structures, by thinning the CdS window layer to under 0.1 microns, and by controlling the uniformity of deposition over large (>4000 cm^2) areas. The films can be deposited by chemical and physical vapor deposition, by electrodeposition, and by sputtering.

Silicon Film: These projects perform applied research on processes for the deposition of relatively thin crystalline silicon (50-100 microns) amenable to exceptionally high throughput rates. Methods include orthogonally directed recrystallization of silicon powder on inexpensive ceramic substrate.

Keywords: Amorphous Silicon, Amorphous Materials, Polycrystalline Films, Polycrystalline Thin Films, Copper Indium Diselenide, Cadmium Telluride, Thin-Film Photovoltaics, Crystalline Silicon Films, Film Silicon,

Silicon Recrystallization, Rapid Thermal Annealing, Semiconductors, Coatings and Films, Chemical Vapor Deposition, Physical Vapor Deposition, Sputtering, Electrodeposition, Semiconductors, Photovoltaics, Solar Cells, Semiconductors

169. DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS
1,450,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contacts: Sarah Kurtz, 303-384-6475, Martha Symko-Davies, 303-384-6528, 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. 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. Research is focused on precise deposition of layers, elucidation of the properties of the interfacial regions, selection of manufacturable combinations of lattice-matched (and also lattice-mismatched) materials with appropriate bandgaps, and improved understanding of the conduction limiting mechanisms of the materials. Conduction limiting mechanisms are particularly severe in the case of GaInAsN, an otherwise favorable material for use in a four-junction super high efficiency concentrator cell.

Materials are deposited by metal organic chemical vapor deposition, liquid phase epitaxy, and molecular beam epitaxy. NREL has verified a monolithic three-junction III-V concentrator cell at over 37 percent conversion efficiency.

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

170. NANOCRYSTALLINE AND ORGANIC SOLAR CELL MATERIALS
$1,375,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contact: David Ginley, 303-384-6573, Arthur Nozik, 303-384-6603, Arthur Frank, 303-384-6262, Robert McConnell, 303-384-6419

These projects focus on the early development of nanocrystalline films (including dye-sensitized nanocrystalline films of titanium dioxide), photovoltaic devices based on nanocrystal composites, novel nanostructure arrays for potentially very high efficiency solar cells, and heterostructure and tandem organic solar cells for potentially very low cost photovoltaics. Fundamental research explores the physical and chemical mechanisms of these novel photovoltaic materials, and identifies the limits to efficiency and future commercial viability.

Keywords: Organic Solar Cells, Nanocrystalline Films, Nanostructures, Dye-Sensitized Cells, Nanocrystals, Biomemetics, Biomemetic Photovoltaics, Organic Solar Cells, Polymer Solar Cells, Conductive Polymers, Next-Generation Photovoltaics, Third-Generation Photovoltaics, Carrier Relaxation Dynamics, Impact Ionization, Hot Carriers, Thermalization of Hot Carriers, Quantum Dot Arrays

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

171. MATERIALS AND DEVICE CHARACTERIZATION
$6,780,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contact: Pete Sheldon, 303-384-6533

These projects measure and characterize material and device properties. Activities include surface, interface, compositional, and electro-optical characterization of photovoltaic materials, and characterization of cell and module performance. Such measurements allow study of critical material and cell parameters such as impurities, layer mismatch, and other defects that limit photovoltaic performance and lifetime. Specific techniques include deep level transient spectroscopy, electron beam induced current, secondary ion mass spectroscopy, X-ray photoelectron spectroscopy, scanning electron microscopy and scanning transmission electron microscopy, Auger spectroscopy, Fourier-transform based measurements (e.g., FT-Raman and FTIR), 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, Photovoltaic Material Characterization

172. MATERIALS STRUCTURE AND COMPOSITION
$1,950,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contacts: Alex Zunger, 303-384-6672, John Benner, 303-384-6496, Robert McConnell, 303-384-6419

These projects support the fundamental and exploratory research needed for advancement of PV technologies in the long term—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 quaternary alloys, e.g., GaInAsN, 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, Ternary Semiconductors, Quaternary Semiconductors, Nanostructured Materials

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

173. MATERIALS IMPROVEMENT FOR HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS
$2,360,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contacts: John Benner, 303-384-6496, Pete Sheldon, 303-384-6533, Robert McConnell, 303-384-6419
Golden Field Office: Glenn Doyle, 303-275-4706

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 on crystalline silicon cell fabrication processes, including rapid thermal processing (RTP), is done at the DOE Center of Excellence (COE) in Photovoltaics at Georgia Institute of Technology. One of the major goals of the COE effort is to develop an RTP-based, screen-printed-contact, photolithography-free, protocol that will yield 18 percent efficient 100 cm^2 cells on crystalline material. This will allow complete fabrication of a high-efficiency silicon cell—from wafer blank to finished cell—in under two hours. Crystalline silicon materials for achieving this goal include multicrystalline silicon made by the Heat Exchange Method (HEM), ribbon material, and single-crystal silicon made by the Czochralski method.

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

174. INSTRUMENTATION AND FACILITIES
$900,000
DOE Contact: Jeffrey Mazer, 202-586-2455
NREL Contact: Pete Sheldon, 303-384-6533, Larry Kazmerski, 303-384-6600
SNL Contact: Joe Tillerson, 505-844-1806

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

There was planning work for the new Science & Technology Facility (S&TF) to be built next to the SERF Building at NREL. However, major funding for, and construction of, this facility will occur in the three fiscal years 2005-2007.

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

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

	FY 2004
OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION - GRAND TOTAL	$33,650,000
HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS	$33,650,000
Second Generation Wire Development	12,050,000
Systems Technology - Partnerships with Industry	16,360,000
Strategic Research	5,240,000

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

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

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

The primary functions of OETD are:

- research and development
- modeling and analysis
- electricity import/export authorization
- power marketing liaison

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

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

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

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

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

In FY 2004, the Superconductivity Program’s parent organization was the Office of Electric Transmission and Distribution (OETD). OETD’s mission is to lead a national effort to help modernize and expand America’s electric delivery system to ensure a more reliable and robust electricity supply, as well as economic and national security.

Several strategic guidance documents support the activities of the Superconductivity Program:

National Energy Policy (2001) - Expand the Department's research and development on transmission reliability and superconductivity

National Transmission Grid Study (2002) - Accelerate the development and demonstration of its technologies including high-temperature superconductivity

President's Council of Advisors on Science and Technology (2002) - DOE-funded research on superconductivity should be increased with a continuing focus on technologies that will reduce the cost of superconductive wire, transformers, generators, and motors, together with supporting technologies such as high-performance cryogenics.

Grid 2030 (2003) - By 2020, HTS generators, transformers and cables will make a significant difference, long distance superconducting transmission cables, by 2030 will complete a national (or continental) superconducting backbone.

The FY 2004 annual operating budget of High Temperature Superconductivity for Electric Systems Program was approximately equal to the prior year's budget. This relatively flat funding profile has stalled new initiatives and research thrusts. The result was somewhat lower spending on capital equipment for national laboratories and industry-led demonstration projects. Results that will be presented at the Peer Review in the summer of 2005 will determine what, if any, effect the actual operating budget will have in achieving milestones for the long term commercialization of the technology.
DOE Contact: Jim Daley, 202-586-1165

175. SECOND GENERATION WIRE DEVELOPMENT
$12,050,000
National Laboratories:
Argonne National Laboratory Contact: George Crabtree, 630-252-5509
Brookhaven National Laboratory Contact: Mas Suenaga, 631-344-3518
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 Howe, 508-621-4209
SuperPower Contact: Phillip Pellegrino, 518-346-1414
Oxford Superconducting Technology Contact: Seung Hong, 732-541-1300
MicroCoating Technologies Contact: Todd Polley, 678-287-2421

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

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

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

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

Project subtasks are as follows:

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

Thick HTS films - Teams made significant progress in 2004 in the development of thick HTS films. The films will be deposited on flexible tapes containing oxide buffer layers deposited by IBAD. Efforts continued to include analysis of electrical flow in thick films, and the development of new diagnostic techniques for identifying "bottlenecks" in the superconductors.

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

IBAD Research - Enhanced performance and reproducibility of IBAD MgO coated conductors were achieved. IBAD MgO offers significant cost benefits compared to IBAD YSZ. In 2004, improvements were made in reel-to-reel substrate electropolishing, developing a new IBAD nucleation layer (Y_2O_3), processing refinements, developing a new buffer layer ($SrRuO_3$), and improving MgO texture resulting in critical current density equal to single crystal substrates.

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

Industrial Scale-Up - The Program in partnership with the Air Force (Title III) will administer a competition for industry to investigate and develop the methods and expertise to begin scaling up coated conductor fabrication processes. Each process will be investigated for its potential to produce high quality, uniform conductors, acceptable economics, process limitations (including time constraints), and long term market potential. Some processes being researched in conjunction with national laboratories are "batch techniques" and questions how to configure their processes for continuous production need to be addressed.

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

176. SYSTEMS TECHNOLOGY - PARTNERSHIPS WITH INDUSTRY
$16,360,000

A goal of the Superconductivity Program is to develop continuous-duty, high capacity electric power equipment that has significant advantages (efficiency, size, weight) compared to equipment now in use. The Superconductivity Partnerships 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.

Project subtasks are as follows:

<u>SPI Readiness Review Program</u>
ORNL Contact: Mike Gouge, 865-576-4467

The focus of this project is on collaboration with the SPI team to identify potential failure modes; issues involving cryogenic temperatures, vacuum and high voltage dielectrics are a major concern. Expertise is obtained as needed from national laboratories, universities, and consultants. The program began in March 2003 and the objective for 2004 is to provide at least one review of all active SPI projects.

<u>Triaxial Cold Dielectric Superconducting Distribution Cable</u>
Ultera Contact: David Lindsay, 770-832-4916

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

Cold Dielectric Superconducting Distribution Cable (with YBCO segment)
SuperPower Contact: Philip Pellegrino, 518-346-1414

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

Coaxial Cold Dielectric Superconducting Transmission Cable
American Superconductor Contact: Michael McCarthy, 508-621-4380

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

HTS Transformer
ORNL Contact: Bob Hawsey, 865-574-8057

The objective in 2004 of the current Phase II Superconductivity Partnership Initiative (SPI) project with Waukesha Electric Systems (WES), SuperPower, Inc. (SP), and Energy East, is to demonstrate the technical and economic feasibility of HTS transformers of medium (30 MVA) to larger ratings. An alpha-prototype 5/10 MVA, 3-phase, HTS transformer, with primary/ secondary voltage ratings of 24.9/4.2 kV and 100-kV BIL has been designed, fabricated, and tested.

Development of Ultra-Efficient HTS Motor System
Rockwell Automation Contact: Rich Schiferl, 216-261-3644

The purpose of the project is to perform research in eight areas related to commercial viability of industrial motors with high temperature superconducting (HTS) windings. The eight areas were identified based upon the past work that Rockwell Automation had conducted on development and testing of HTS based motors up to and including the laboratory test of a 1600 hp motor.

Cost Effective, Open Geometry Superconducting Magnetic Resonance Imaging (MRI) System
Oxford Contact: Kenneth Marken, 732-541-1300

The purpose in 2004 of this Phase II Superconductivity Partnership Initiative project is to build and operate a prototype Magnetic Resonance Imaging (MRI) system using HTS coils wound from low-cost, dip-coated BSCCO 2212 tape conductor. The planned milestones for FY 2004 were: 1) complete precursor powder manufacturing upgrades; 2) complete prototype conductor processing line; 3) begin conductor fabrication 4) complete design of cryogenics system and magnet.

Design and Development of a 100 MVA HTS Generator
ORNL Contact: Bob Hawsey, 865-574-8057

General Electric's Global Research in Niskayuna, N.Y., will design and develop a 100 MVA class high-temperature superconducting (HTS) generator, with designs through 250 MVA. The HTS rotor will be capable of retrofitting into existing generators. ORNL and LANL have entered into CRADAs with GE to provide assistance in several technology areas.

Development Status of Flywheel Electricity System
Boeing Contact: Mike Strasik, 425-237-7176

The main purpose of this effort is to develop a 10-kWh flywheel energy system based on high-temperature superconducting (HTS) bearings. The first unit developed had a 3-kW motor/generator (M/G). The second unit developed has a 100-kW M/G. This effort started in FY1999. Due to DOE's funding limitations this year, the Boeing project received significantly lower funding than planned, and no funding was available for national laboratory support. Specific objectives for FY 2004 were to complete the manufacturing of all components for the 100 kW/5 kWh UPS flywheel system, test all individual components at full speed, assemble the system, and fully test the UPS flywheel system at Boeing site with technical assistance from Southern California Edison's test personnel.

Waste Water Treatment with Magnetic Separation
LANL Contact: John Bernard, 505-663-5593

DuPont is leading the SPI development of a 500 mm HTS reciprocating magnetic separator. An HTS magnetic separator offers significant operational energy savings compared to conventional copper coil separators. The DuPont business plan calls for the development of new applications of magnetic separation that can benefit from the energy efficiency. After jointly assessing several potential market opportunities, DuPont and LANL agreed to focus on the removal of heavy metals in wastewater using high gradient magnetic separation (HGMS). LANL will work with DuPont to develop an in-situ ferrite formation process that incorporates the heavy metals in a ferrite crystal lattice. The ferrites, having a high magnetic susceptibility, are then readily removed as they pass near a magnetized matrix material.

Matrix Fault Current Limiter
SuperPower Contact: Philip Pellegrino, 518-346-1414

The purpose of this project is to conduct R&D on specified components and provide technical design support to a SuperPower, Inc. (SP) team developing high temperature superconducting (HTS) technology for a Matrix Fault Current Limiter (MFCL). This device incorporates a series-parallel array of bulk HTS elements and inductors in a sub-cooled liquid nitrogen (LN) bath. Transition of the HTS elements into the normal state during a fault drives most of the current into the inductors and leads to a sudden increase in impedance that limits the fault current

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

177. STRATEGIC RESEARCH
$5,240,000
Argonne National Laboratory Contact:
George Crabtree, 630-252-5509
Brookhaven National Laboratory Contact:
Mas Suenaga, 516-282-3518
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 2004. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties. Additionally, Sandia scientists worked on developing high-quality, solution-derived, 123-type superconducting films for coated conductor applications.

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

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

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

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

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

Keywords: Superconducting Tapes, Flux Pinning, Bismuth Conductor

OFFICE OF SCIENCE

	FY 2004
OFFICE OF SCIENCE - GRAND TOTAL	$689,599,712
OFFICE OF BASIC ENERGY SCIENCES	$631,276,000
DIVISION OF MATERIALS SCIENCES AND ENGINEERING	$235,806,000
Theoretical Condensed Matter Physics	18,126,000
Experimental Condensed Matter Physics	42,631,000
Materials Chemistry	40,338,000
Mechanical Behavior and Radiation Effects	13,444,000
X-ray and Neutron Scattering	44,928,000
Structure and Composition of Materials	22,833,000
Physical Behavior	22,148,000
Synthesis and Processing Sciences	12,710,000
Engineering Physics	10,975,000
Experimental Program to Stimulate Competitive Research	7,673,000
DIVISION OF SCIENTIFIC USER FACILITIES	$395,470,000
X-ray and Neutron Scattering Facilities	298,138,000
Nanoscience Centers	97,332,000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH	$48,034,712
TECHNOLOGY RESEARCH DIVISION	$48,034,712
LABORATORY TECHNOLOGY RESEARCH PROGRAM	$610,100
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$413,400
Advanced Processing Techniques for Tailored Nanostructures in Rare-Earth Permanent Magnets	225,200
Low-Cost, High-Performance YBCO Conductors	188,200
DEVICE OR COMPONENT FABRICATION, BEHAVIOR, OR TESTING	$196,700
Nanofabrication of Advanced Diamond Tools	196,700
SMALL BUSINESS INNOVATION RESEARCH PROGRAM	$43,926,813
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$11,622,260
FY 2004 PHASE I	$2,996,584
Ceramic Microchannel Plates with Angular-Biased Channels	99,999
100Gb/s-1Tb/s Data Communications, Via Cost-Effective Transceivers Based on Monolithic Integration of WDM Lasers and Photodetectors with Ultra-Compact Wavelength Mux/Demux	100,000
Novel Silica Aerogel Panels as Radiators for Cherenkov Detectors	99,939
CdZnTe Detector Advancement Through Defect Reduction	100,000
Single Crystal Molybdates for Neutrinoless Double Beta Decay Experiments	100,000
A Device to Measure Low Levels of Radioactive Contaminants in Ultra-Clean Materials	100,000
Discovery of Dense Ce Activated Scintillators for SPECT and PET by High Throughput Screening Method	100,000

OFFICE OF SCIENCE (continued)

	FY 2004
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
FY 2004 PHASE I (continued)	
A Detector for Combined SPECT/CT	100,000
A New Ceramic Scintillator for Neutron Detection	100,000
A High Purity Silicon X-ray Detector	100,000
Nanostructured Non-Carbonaceous Anode and Separator for High Energy and Power Density Rechargeable Li-Ion Batteries	99,990
Novel, Redox Stabilized Li-Ion Rechargeable Cell	100,000
Low-Cost, Environmentally Benign, High Specific Power Manganese Dioxide-Carbon Pseudocapacitors for Hybrid Vehicles	99,904
Composite Anode Interlayers for Lithium Batteries with Stable Anode-Electrolyte Interfaces Under High Charging Current Densities	99,997
Nanocomposite Polymers for Smart Window Films	98,028
Catalytic Membrane Reactors: Next Generation Mixed Conducting Membranes	99,997
Enhancing Charge Injection and Device Integrity in Organic LEDs	99,915
High Performance, Silicon Nanocrystal-Enhanced Organic Light Emitting Diodes for General Lighting	99,993
Zinc Oxide Based Light Emitting Diodes	100,000
Transparent, Highly-Efficient, White OLEDs for Lighting Applications	100,000
Development of Polymer Processing Techniques for Dramatic Cost Reduction of Large Core Plastic Optical Fiber, for Use with Advanced, High Intensity Discharge (HID) Distributed Accent Lighting System	99,245
High Efficiency ZnO-Based LEDs on Conductive ZnO Substrates for General Illumination	100,000
Novel Microporous Membranes for Hydrogen Separation from Hydrotreater Recycle Gas	100,000
Metallic Foam-Based Membranes for Hydrogen Separation/Purification	99,987
Compact Heat Exchanger for Micro-Turbine-Based Cooling, Heating, and Power	99,816
Novel Heat Exchangers with Enhanced Surface	100,000
Polymer-Derived Silicon Carbide Membranes for Hydrogen Separation	99,839
Composite, High-Temperature Seals for Gas Separation Membrane Devices	99,936
Advanced SiC-Based Membranes for Hydrogen Separation	100,000
Optimization of Metal Alloy for High Pressure Hydrogen Separation Membrane	99,999
FY 2004 PHASE II (FIRST YEAR)	$4,133,277
Fast, High Resolution Pet Detector	375,000
A Remote and Affordable Detection System for Cr(VI) in Groundwater	374,918
Nanoscale Inorganic Ion-Exchange Films for Enhanced Electrochemical Heavy Metal Detection	374.997
A GEM of a Neutron Detector	361,858
Novel Light Extraction Enhancements for OLED Lighting	375,000
Novel, Low - Cost Technology for Solid State Lighting	374,976
Low-Cost Fabrication of Inertial Fusion Energy Capsule Supports	374,850
New N+ Contact for Germanium Strip Detectors	375,000
Geiger Photodiode Array Readouts for Scintillating Fiber Arrays	367,510
A High Current Density, Low Magnetization, Tubular Filamented Nb_3Sn Superconductor	99,263
Development of Internal-Tin Nb/Sn Strand for High Field Accelerator Dipole Applications	300,000
Engineered Ceramic Composite Insulators for High Field Magnet Applications	379,905

OFFICE OF SCIENCE (continued)

	FY 2004
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
FY 2004 PHASE II (SECOND YEAR)	$4,492,399
Perovskite/Oxide Composites as Mixed Protonic/Electronic Conductors for Hydrogen Recovery in IGCC Systems	374,909
Highly Textured Composite Seals for SOFC Applications	375,000
Biomimetic Membrane for Carbon Dioxide Capture from Flue Gas	369,372
Low-Cost Nanoporous Sol Gel Separators for Lithium-Based Batteries	288,552
New Solid State Lighting Materials	374,907
Transformer Ratio Enhancement Experiment for Next Generation Dielectric Wakefield Accelerators	300,000
High Current Density (Jc), Low AC Loss, Low Cost Internal-Tin Superconductors	374,911
Microwave Component Fabrication using the Fast Combustion Driven Compaction Process	374,835
Micro-Photomultiplier Array	360,370
Electrically Medicated Microetching Manufacturing Process to Replace Emersion and Spray Etching	374,960
Separation and Enrichment of Xenon in Air	299,939
High Performance Thermo-Electrically-Cooled LWIR Mercury Cadmium Telluride Detectors	250,000
VEGF-Based Delivery of Boron Therapeutics	374,644
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$7,566,387
FY 2004 PHASE I	$699,219
Innovative, Low Cost, Radiation-Resistant Fusion Magnet Insulation	99,997
Development of a Canonical Approach to Liquid Metal MHD Computations and Experiments	100,000
Hybrid Spinel Composites: Unique Radiation Resistant Refractories	99,914
Novel, High Energy Density Intermetallic Anode Material for Li-Ion Batteries	100,000
Self-Cleaning Surfaces with Morphology Mimicking Superhydrophobic Biological Surfaces	99,308
Investigation of $(CaO)_x(Al_2O_3)_x$ for Thermal Insulation and Molten Aluminum Contact	100,000
Use of Amended Silicates for Multi-Pollutant Control in Gasifiers	100,000
FY 2004 PHASE II (FIRST YEAR)	$6,117,194
A Design of a New Readout Sensor for Spect	375,000
High Performance Pet Detector	375,000
Electrodecontamination for Mitigation of Airborne Contamination	374,999
Evaluation of a Novel Magnetic Activated Carbon Process for Gold Recovery	184,692
Tailorable, Environmental Barrier Coatings for Super- Alloy Turbine Components in Syngas	374,802
Hot Section Material Systems Testing and Development for Advanced Power Systems	368,057
SiCN High Temperature Microelectromechanical Systems (MEMS) Sensor Suite	374,986
Enhanced Performance Carbon Foam Heat Exchanger for Power Plant Cooling	365,060
Dehydration of Natural Gas	374,972
High Pressure Economical Process for Treating Natural Gas	375,000
Novel Fischer-Tropsch Reactor	374,992

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	FY 2004
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
FY 2004 PHASE II (FIRST YEAR) (continued)	
Innovative Inorganic Fusion Magnet Insulation Systems	374,996
Aluminum Nitride Radio Frequency Windows	375,000
A Novel Design for CZT Gamma Ray Spectrometers	375,000
Some Improved Methods of Introducing Additional Elements into Internal-tin Nb_3Sn	324,786
Fast X-Band Phase Shifter	375,000
Near Net Shape Manufacturing Using Combustion Driven Compaction	374,852
FY 2004 PHASE II (SECOND YEAR)	$749,974
Multilayer Composite Membranes for Upgrading Acid-Rich Natural Gas	375,000
Stabilized Lithium Manganese Oxide Spinel Cathode for High Power Li-Ion Batteries	374,974
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$15,051,811
FY 2004 PHASE I	$2,787,481
Lower Cost Nb3Sn Internal-Tin Strand for ITER Fusion Project	100,000
Flowing Liquid Lithium Walls Using Engineered Surfaces	100,000
Ternary Nb-Ti-Ta Alloys for High Field 2 K Applications—Alloy Selection and Process Optimization	100,000
High Superconductor Fraction, High Engineering Critical Current Density Bi-2212/Ag Wires Fabricated by Ultrasonic Wire Drawing	100,000
Increase Piece Length and Reduce Cost of A15 Superconductor Wire by Eliminating Wire Drawing Breakage	100,000
Moldable Ceramic Composites for High Field Magnet Applications	99,999
Low Loss Ferroelectric Material Development for Accelerator Applications	98,114
Advanced Fluoropolymer Vessels for Ultra-Clean Ionization and Scintillation Detectors	100,000
Coaxial Energetic Ion Depostition of Superconducting Coatings on Copper RF Cavities for Particle Accelerators	99,985
A Method for Electroforming Copper with Ultra-Low Levels of Radioactivity	100,000
Novel Micro-Nanoprobes and Detection Method for Biomedical Applications	97,496
Ceramic Composite Fuel Encapsulation in High Efficiency, Advanced Pebble-Bed Gas Reactors	100,000
Anode Electrolyte Nanocomposites as Alternative to Carbonaceous Anode Materials	99,986
Polythiophosphonate Electrolytes for Rechargeable Magnesium Batteries	99,992
Lithium Ion-Channel Polymer Electrolyte for Lithium Metal Anode Rechargeable Batteries	100,000
Low Cost, High Performance PPSA-Based PEM Fuel Cell Membranes	99,135
Oxidation Protection via Nanocrystalline Coatings	100,000
Shape Memory Polymer Nanocomposites	99,996
Novel Nanoscale Intermetallic Fuel Cell Catalyst Materials and Processing	94,993
Novel, Active Layer Nanostructures for White Light Emitting Diodes (LEDS)	99,717
High Efficiency Nanocomposite White Light Phosphors	99,891
New, Efficient Nanophase Materials for Blue and Deep Green Light-Emitting Diodes	100,000
Composite Metal-Ceramic Hydrogen Separation Membranes	99,999
High Temperature Pervaporation Membrane and Process	100,000

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	FY 2004
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
FY 2004 PHASE I (continued)	
Functionally Graded Aluminum Nitride - Oxide Coatings for Hot Pipe Protection	99,999
Development of Solar Grade (SoG) Silicon	99,928
An Innovative Technique of Preparing Solar Grade Silicon Wafers from Metallurgical Grade Silicon by In-Situ Purification	100,000
Light-Weight Nanocrystalline Hydrogen Storage Materials	98,251
FY 2004 PHASE II (FIRST YEAR)	$6,352,306
Al(In)GaN-Based, High-Electron Mobility Transistors (HEMTs) on SiC for High-Power Radar Applications	375,000
Cell-Free Protein Synthesis for High-Through-Put Proteomics	367,649
Low-Cost Automatic Tool Fixturing Based on Dexterous Robotic Hand	375,000
Solid-State Thermal-Neutron Detector Based on Boron-Doped a-Se Stabilized Alloy Films	374,946
New, Stable Cathode Materials for OLEDs	374,912
Novel Lower-Voltage OLEDs for Higher-Efficiency Lighting	375,000
$LiFePO_4$ Cathode Material Designed for Use in Lithium-Ion Batteries with Application to Electric and Hybrid-Electric Vehicles	374,902
Metal Oxide Catalyst for Methyl Ethyl Ketone Production via One-Step Oxidation of n-Butane	374,995
Low Cost and High Performance, Polymer Nanocomposite, Specialty Industrial Coatings	374,994
Industrial Nano Material Components with High Temperature Corrosion and Wear Resistance Performance for Energy Savings	374,998
High Temperature-Stable Membrane Electrode Assemblies for Fuel Cells Fabricated via Ink Jet Deposition	375,000
Cost Effective Improved Refractory Materials for Gasification Systems	374,117
Advanced Net-Shape Insulation for Solid Oxide Fuel Cells	374,959
High-Performance, Plasticization-Resistant Membranes for Natural Gas Separations	374,997
Cost Effective Fischer-Tropsch Technology	360,839
Nanocomposite Dielectric Materials for High Frequency Applications	374,998
Very Large, High Gain APDs for Particle Physics	375,000
FY 2004 PHASE II (SECOND YEAR)	$5,912,024
Embedded Sensors in Turbine Systems by Direct Write Thermal Spray Technology	349,881
Catalyst to Improve Small-Scale Claus Plants	375,000
LSGM Based Composite Cathodes for Anode Supported, Intermediate Temperature (600-800 degrees C) Solid Oxide Fuel Cells (SOFC)	249,634
Metal Oxide Catalyst for Methacrylic Acid Preparation via One-Step Oxidation of Isobutane	374,998
P-Type ZnO Films	375,000
An Advanced Cathode Material for Li-Ion Battteries	374,580
Three-Dimension Woven Carbon-Glass Hybrid Wind Turbine Blades	333,188
Feasibility of Cost Effective, Long Length, BSCCO 2212 Round Wires, for Very High Field Magnets, Beyond 12 Tesla at 4.2 Kelvin	311,806
Growth of a New, Fast Scintillator Crystal for Nuclear Experiments	374,423

OFFICE OF SCIENCE (continued)

	FY 2004
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
FY 2004 PHASE II (SECOND YEAR) (continued)	
A New Scintillator for Gamma Ray Spectroscopy	375,000
Diamond Windows for High Power Microwave Transmission	373,149
Radiation Resistant Insulation with Improved Shear Strength for Fusion Magnets	374,707
Nanostructured Tungsten for Improved Plasma Facing Component Performance	375,000
Low Cost Materials for Neutron Absorption in Generation IV Nuclear Power Systems	299,750
High Resolution Gamma Ray Spectrometer for Nuclear Non-Proliferation	375,000
Growth of a New Mid-IR Laser Crystal	374,709
Induim Arsenide Antimonide Very Long Wavelength Photodiodes for Near Room Temperature Operation	246,199
INSTRUMENTATION AND FACILITIES	$8,940,292
FY 2004 PHASE I	$300,000
Novel Scintillator for Nuclear Physics Studies	100,000
Ultra-Low Background Alpha Activity Counter	100,000
Ultra-Sensitive, Compact Mid-Infrared Spectrometer for Airborne and Ground-Based Atmospheric Monitoring	100,000
FY 2004 PHASE II (FIRST YEAR)	$7,271,189
Situational Awareness Monitor for Nuclear Events	374,999
Low-Noise Borehole Triaxial Seismometer	359,360
Compact, Short-Pulse Laser Source for Active Imaging Systems	374,996
Advanced, Aerosol Mass Spectrometer for Aircraft Measurement of Organic Particulate Matter	375,000
Cavity Attenuation Phase Shift Spectroscopic Detection of Nitrogen Dioxide	375,000
Novel Ultrasensitive Instrumentation for Trace Gas Measurements in the Field	311,652
Innovative Carbon Dioxide Sensor Based on Cavity Ringdown	373,834
High Precision CO_2 Sensor for Balloon Sonde Atmospheric Measurements	372,333
A Down-Hole Probe for Real-Time Ore Grade Assessment in “Look Ahead” Mining	375,000
Development of HSTAT for HVAC Health Status and Control	375,000
An Extremely High Power, Field-Coupled, Low-Loss RF Transmission Line for SRF Cavities	369,979
Magnetized Electron Transport in the Proposed Electron Cooling Section of the Relativistic Heavy Ion Collider	374,957
Ultra High Speed Analog to Digital Converter with Ternary Digital Output	375,000
High Precision, Integrated Beam Position and Emittance Monitor	374,999
Six-Dimensional Beam Cooling in a Gas Absorber	375,000
High-Power Radio Frequency Window	97,308
Hybrid Modulator Upgrade	232,839
NLC Marx Bank Modulator	373,081
Quasi-Optical 34-GH_z Radio Frequency (RF) Pulse Compressor	375,000
A Hydrostatic Processing Facility for Superconducting Wire	330,856
Novel Magnetometer for Quadrupole and Dipole Magnetic Measurements	324,996

OFFICE OF SCIENCE (continued)

	FY 2004
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES (continued)	
FY 2004 PHASE II (SECOND YEAR)	$1,369,103
An Inexpensive, Efficient Neutron Monochromator	375,000
High Gain, Fast Scan, Broad Spectrum, Parallel Beam Wavelength Dispersive X-Ray Spectrometer for SEM	273,093
Advanced X-Ray Detectors for Transmission Electron Microscopy	375,000
Using Convergent Beams for Small-Sample, Time-of-Flight Neutron Diffraction	346,010
MATERIALS STRUCTURE AND COMPOSITION	$746,063
FY 2004 PHASE I	$299,892
Microstructural Refinement of Tantalum for Superconductor Diffusion Barrier Applications	99,916
"Metal Rubber" Nanostructured Materials	100,000
High Extraction Luminescent Material Structures for Solid State Light Emitting Diodes	99,976
FY 2004 PHASE II (SECOND YEAR)	$446,171
Development of a New, Low Frequency, Rf-Focused Linac Structure	446,171
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM	$3,497,799
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$1,499,213
FY 2004 PHASE I	$699,225
Solid State and Resistance Joining Technologies for Fusion Energy Systems	100,000
Advanced Plasma Gun Development for Simulating Edge-Localized-Mode Plasma Disruptions with Application to Free Surface Flowing Liquid Metal PFCs	99,897
Thinner Silicon Detectors and Novel Interconnections for Robust High Energy Physics Detectors	99,432
Ultra-Trace Molecular Detection Instrumentation Based on Aerosol Nucleation with Rapid Preconcentration and Separation	100,000
Novel Photocatalytic Energy Converter for Nuclear Safeguards Applications	99,896
A Compact, In-Situ Instrument for Organic Acids	100,000
Efficient Nanotube-Based OLEDs	100,000
FY 2004 PHASE II (FIRST YEAR)	$375,000
Engineered Tungsten Surfaces for IFE Dry Chamber Walls	375,000
FY 2004 PHASE II (SECOND YEAR)	$424,988
Carbon Fiber Composite Aeroelastically Tailored Rotor Blades for Utility-Scale Wind Turbines	424,988

OFFICE OF SCIENCE (continued)

	FY 2004
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$250,000
FY 2004 PHASE II (SECOND YEAR)	$250,000
Hydroforming of Light Weight Components from Aluminum and Magnesium Sheet and Tube	250,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,648,586
FY 2004 PHASE I	$598,640
Fabrication of Chemically Doped, High Upper Critical Field Magnesium Diboride Superconducting Wires	99,683
Nanocomposite Membranes for High Temperature Proton Exchange Membrane Fuel Cells	99,901
Polymer Composite Barrier System for Encapsulating LEDs	99,349
Surface Modification of Nanoporous Zeolite Pervaporation Membranes for Enhanced Biomass Product Recovery	99,760
Bulk Nanophase High Transition Temperature Shape Memory Alloys for Novel Waste Heat Recovery Systems	100,000
Conformal Power Harvesting Microstructures	99,947
FY 2004 PHASE II (FIRST YEAR)	$749,946
Nanostructured Polymeric Heterogeneous Catalyst for Industrial Applications	375,000
Novel Approach Toward High Performance Energetic Rays Detection	374,946
FY 2004 PHASE II (SECOND YEAR)	$300,000
Waveshifters and Scintillators for Ionizing Radiation Detection	300,000
INSTRUMENTATION AND FACILITIES	$100,000
FY 2004 PHASE I	$100,000
High Brightness Neutron Source for Radiography	100,000
OFFICE OF FUSION ENERGY SCIENCES	$9,000,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$9,000,000
Vanadium Alloy and Insulating Coating Research	1,500,000
Theory and Modeling	1,700,000
Ferritic/Martensitic Steel Research	2,300,000
SiC/SiC Composites Research	1,500,000
Plasma Facing Materials Research	2,000,000

OFFICE OF SCIENCE (continued)

	FY 2004
OFFICE OF BIOLOGICAL & ENVIRONMENTAL RESEARCH	$1,289,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,289,000
Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes	79,000
Physical, Chemical and Structural Evolution of Zeolite-Containing Waste Forms Produced from Metakaolinite and Calcined HLW	50,000
Investigating Ultrasonic Diffraction Grating Spectroscopy and Reflection Techniques for Characterizing Slurry Properties	170,000
Chemistry of Actinides in Molten Glasses and Its Correlation to Structural Performance of Solid Glasses: Filling the Knowledge Gap	140,000
Stability of High Level Radioactive Waste Forms	290,000
Assessing the State and Distribution of Radionuclide Contamination in Concrete: An Experimental and Modeling Study of the Dynamics of Contamination	300,000
Underground Corrosion After 32 Years: A Study of Fate and Transport	260,000

OFFICE OF SCIENCE

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

- Office of Basic Energy Sciences - Division of Materials Sciences and Engineering
- Office of Basic Energy Sciences - Division of Scientific User Facilities
- Office of Advanced Scientific Computing Research - Division of 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 and Engineering conducts a broad program of materials research to increase the understanding of phenomena and properties important to materials behavior that will contribute to meeting the needs of present and future energy technologies. The Division supports fundamental research in materials at DOE national laboratories and plans, constructs, and operates national scientific user facilities needed for materials research. In addition, the Division funds over 230 grants, mostly with universities, on a wide range of topics in materials research. Fundamental materials research is carried out at eleven DOE laboratories: Ames Laboratory at Iowa State University, Argonne National Laboratory, Brookhaven National Laboratory, Idaho National Environmental and Engineering Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories in New Mexico and California, and the Stanford Synchrotron Radiation Laboratory. The laboratories also conduct significant research activities for other DOE programs such as Energy Efficiency, Fossil Energy, Nuclear Energy, Environmental Management and Defense Programs. The Division of Materials Sciences and Engineering also funds the University of Illinois Frederick Seitz Materials Research Laboratory. Summaries of the laboratory portion of the program and an interim listing of FY 2004 grants are available on the World Wide Web at the following address: http://www.science.doe.gov/bes/dms/Research_Programs/research_program.htm.

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

Theoretical Condensed Matter Physics

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

An important facilitating component is the Computational Materials Science Network (CMSN), which enables groups of scientists from DOE laboratories, universities, and (to a lesser extent) industry to address materials problems requiring larger-scale collaboration across disciplinary and organizational boundaries. The FY 2004 funding for this program is $18,126,000 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 2004 funding for this program is $42,631,000 and the DOE contact is James Horwitz, 301-903-4894.

Materials Chemistry and Biomolecular Materials

This activity broadly supports basic, exploratory research on the design, synthesis, characterization, and properties of novel materials and structures. The general focus is on the chemical aspects of complex and collective phenomena that give rise to advanced materials. The portfolio emphasizes solid-state chemistry, surface and interfacial chemistry, and materials that underpin many energy-related areas such as batteries and fuel cells, catalysis, friction and lubrication, energy conversion and storage, membranes, electronics and sensors, and materials aspects of environmental chemistry. It includes investigation of novel materials such as low-dimensional solids, self-assembled monolayers, cluster and nanocrystal-based materials, conducting and electroluminescent polymers, organic superconductors and magnets, complex fluids, hybrid materials, biomolecular materials and solid-state neutron detectors. There is an increased emphasis on the synthesis of new materials with nanoscale structural control and taking advantage of unique material properties that originate at the nanoscale. In this regard, addition of a new Program Manager (A. M. K.) for Biomolecular Materials has added a new dimension to the scope of Materials Chemistry research activity. Significant research opportunities exist at the biology/materials science interface since the world of biology offers time-tested strategies and models for the design and synthesis of new materials—composites and molecular assemblies with unique properties and specific functions. A wide variety of experimental techniques are employed to characterize these materials including X-ray photoemission and other spectroscopies, scanning tunneling and atomic force microscopies, nuclear magnetic resonance (NMR), and X-ray and neutron reflectometry. The program also supports the development of new experimental techniques such as high-resolution magnetic resonance imaging (MRI) without magnets, neutron reflectometry, and surface force apparatus in combination with various spectroscopies. The FY 2004 funding for this program is $40,338,000 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 noncrystalline phase), understand mechanisms of radiation damage, predict and learn how to suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by ion implantation. The FY 2004 funding for this program is $13,444,000 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 2004 funding for this program is $44,928,000 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 2004 funding for this program is $22,833,000 and the DOE contact is Jane Zhu, 301-903-3811.

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 2004 funding for this program is $22,148,000 and the DOE contact is Yok Chen (acting), 301-903-4174.

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 2004 funding for this program is $12,710,000 and the DOE contact is Tim Fitzsimmons, 301-903-9830.

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 2004 funding for this program is $10,975,000 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, 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 2004 funding for this program is $7,673,000 and the DOE contact is Matesh Varma, 301-903-3209.

DIVISION OF SCIENTIFIC USER FACILITIES

X-ray and Neutron Scattering Facilities

This activity supports the operation of four synchrotron radiation light sources and three neutron scattering facilities. These are: the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory; the Advanced Photon Source (APS) at Argonne National Laboratory; the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory; the Stanford Synchrotron Radiation Laboratory (SSRL) at Stanford Linear Accelerator Center; the High Intensity Flux Reactor (HFIR) at Oak Ridge National Laboratory; the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory; and the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory. Under construction is the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, which is a nextgeneration short-pulse spallation neutron source that will be significantly more powerful than the best spallation neutron source now in existence—ISIS at the Rutherford Laboratory in England. On the drawing board is the Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center, which is a free-electron laser that will provide laser-like radiation in the X-ray region of the spectrum that is 10 orders of magnitude greater in peak power and peak brightness than any existing coherent Xray light source. The FY 2004 funding for this program is $298,138,000 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 nanofabrication 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 2004 funding for this program is $97,332,000 and the DOE contacts are Kristin A. Bennett, 301-903-4269 and Altaf Carim, 301-903-4895.

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

TECHNOLOGY RESEARCH DIVISION

LABORATORY TECHNOLOGY RESEARCH PROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, OR FORMING

178. ADVANCED PROCESSING TECHNIQUES FOR TAILORED NANOSTRUCTURES IN RARE-EARTH PERMANENT MAGNETS
$225,200
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

179. LOW-COST, HIGH-PERFORMANCE YBCO CONDUCTORS
$188,200
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

180. NANOFABRICATION OF ADVANCED DIAMOND TOOLS
$196,700
DOE Contact: Samuel J. Barish, 301-903-2917
LBNL Contact: Othon Monteiro, 510-486-6159

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

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

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

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

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2004 PHASE I

Ceramic Microchannel Plates with Angular-Biased Channels - DOE Contact Michael P. Saul Gonzalez (301) 903-2359; Synkera Technologies, Inc. Contact Dr. Stephen S. Williams, (720) 494-8401

100Gb/s-1Tb/s Data Communications, Via Cost-Effective Transceivers Based on Monolithic Integration of WDM Lasers and Photodetectors with Ultra-Compact Wavelength Mux/Demux - DOE Contact Thomas Ndousse-Fetter, (301) 903-9960; Optonet, Inc. Contact Dr. Seng-Tiong Ho, (224) 588-0958

Novel Silica Aerogel Panels as Radiators for Cherenkov Detectors - DOE Contact Blaine Norum, (301) 903-4398; Aspen Aerogels, Inc. Contact Mr. Patrick J. Piper, (508) 691-1150

CdZnTe Detector Advancement Through Defect Reduction - DOE Contact Blaine Norum, (301) 903-4398; Fermionics Corporation Contact Dr. Muren Chu, (805) 582-0155

Single Crystal Molybdates for Neutrinoless Double Beta Decay Experiments - DOE Contact Blaine Norum, (301) 903-4398; Integrated Photonics, Inc. Contact Dr. Vincent J. Fratello, (908) 281-0191

A Device to Measure Low Levels of Radioactive Contaminants in Ultra-Clean Materials - DOE Contact Blaine Norum, (301) 903-4398; Reeves & Sons, LLC Contact Mr. James H. Reeves, (509) 943-1653

Discovery of Dense Ce Activated Scintillators for SPECT and PET by High Throughput Screening Method - DOE Contact Dean Cole, (301) 903-3268; Ls Technologies, Inc. Contact Dr. J. Q. Lin, (510) 651-1329

A Detector for Combined SPECT/CT - DOE Contact Dean Cole, (301) 903-3268; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 668-6800

A New Ceramic Scintillator for Neutron Detection - DOE Contact Helen Kerch, (301) 903-2346; Alem-RMD Joint Venture Contact Dr. Gerald Entine, (617) 668-6800

A High Purity Silicon X-ray Detector - DOE Contact Dean Miller, (630) 252-4108; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 668-6800

Nanostructured Non-Carbonaceous Anode and Separator for High Energy and Power Density Rechargeable Li-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Evionyx, Inc. Contact Mr. Michael Chang, (914) 798-7269

Novel, Redox Stabilized Li-Ion Rechargeable Cell - DOE Contact Jim Barnes, (202) 586-5657; Farasis Energy, Inc. Contact Dr. Keith D. Kepler, (510) 864-4800

Low-Cost, Environmentally Benign, High Specific Power Manganese Dioxide-Carbon Pseudocapacitors for Hybrid Vehicles - DOE Contact Jim Barnes, (202) 586-5657; Foster-Miller, Inc. Contact Dr. Richard M. Wiesman, (781) 684-4242

Composite Anode Interlayers for Lithium Batteries with Stable Anode-Electrolyte Interfaces Under High Charging Current Densities - DOE Contact Jim Barnes, (202) 586-5657; Materials and Systems Research, Inc. Contact Dr. Dinesh K. Shetty, (801) 530-4987

Nanocomposite Polymers for Smart Window Films - DOE Contact Charles Russomanno, (202) 586-7543; Wavefront Technology, Inc. Contact Mr. Joel Peterson, (562) 634-0434

Catalytic Membrane Reactors: Next Generation Mixed Conducting Membranes - DOE Contact Charles Russomanno, (202) 586-7543; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 530-0263

Enhancing Charge Injection and Device Integrity in Organic LEDs - DOE Contact Ryan Egidi, (304) 285-0958; Agiltron, Inc. Contact Dr. Lei Zhang, (978) 694-1006

High Performance, Silicon Nanocrystal-Enhanced Organic Light Emitting Diodes for General Lighting - DOE Contact James Brodrick, (202) 586-1856; Innovalight, Inc. Contact Mr. Paul Thurk, (512) 331-9625

Zinc Oxide Based Light Emitting Diodes - DOE Contact James Brodrick, (202) 586-1856; Materials Modification, Inc. Contact Dr. T. S. Sudarshan, (703) 560-1371

Transparent, Highly-Efficient, White OLEDs for Lighting Applications - DOE Contact James Brodrick, (202) 586-1856; Universal Display Corporation Contact Ms. Janice K. Mahon, (609) 671-0980

Development of Polymer Processing Techniques for Dramatic Cost Reduction of Large Core Plastic Optical Fiber, for Use with Advanced, High Intensity Discharge (HID) Distributed Accent Lighting System - DOE Contact James Brodrick, (202) 586-1856; Fiberstars, Inc. Contact Mr. Roger Buelow, (440) 836-7421

High Efficiency ZnO-Based LEDs on Conductive ZnO Substrates for General Illumination - DOE Contact James Brodrick, (202) 586-1856; ZN Technology, Inc Contact Dr. K. Choo, (714) 989-8880

Novel Microporous Membranes for Hydrogen Separation from Hydrotreater Recycle Gas - DOE Contact Charles Russomanno, (202) 586-7543; Trans Ionics Corporation Contact Dr. Robert C. Schucker, (281) 296-5585

Metallic Foam-Based Membranes for Hydrogen Separation/Purification - DOE Contact Charles Russomanno, (202) 586-7543; Ultramet Contact Mr. Craig N. Ward, (818) 899-0236

Compact Heat Exchanger for Micro-Turbine-Based Cooling, Heating, and Power - DOE Contact Ronald J. Fiskum, (202) 586-9154; Altex Technologies Corporation Contact Dr. Mehdi Namazian, (408) 982-2303

Novel Heat Exchangers with Enhanced Surface - DOE Contact Ronald J. Fiskum, (202) 586-9154; MER Corporation (Materials and Electrochemical Research) Contact Dr. Raouf Loutfy, (520) 574-1980

Polymer-Derived Silicon Carbide Membranes for Hydrogen Separation - DOE Contact Richard J. Dunst, (412) 386-6694; Ceramatec, Inc. Contact Mr. Raymond K. Miller, (801) 978-2114

Composite, High-Temperature Seals for Gas Separation Membrane Devices - DOE Contact Udaya Rao, (412) 386-4743; Ceramatec, Inc. Contact Mr. Raymond K. Miller, (801) 978-2114

Advanced SiC-Based Membranes for Hydrogen Separation - DOE Contact Richard J. Dunst, (412) 386-6694; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Optimization of Metal Alloy for High Pressure Hydrogen Separation Membrane - DOE Contact Richard J. Dunst, (412) 386-6694; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 530-0263

FY 2004PHASE II (FIRST YEAR)

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

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

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

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

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

Novel, Low - Cost Technology for Solid State Lighting - DOE Contact Ryan Egidi, (304) 285-0945; Technologies and Devices International, Inc. Contact Dr. V. Dmitriev, (301) 572-7834

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

New N+ Contact for Germanium Strip Detectors - DOE Contact Blaine Norum, (301) 903-4398; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

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

A High Current Density, Low Magnetization, Tubular Filamented Nb_3Sn Superconductor - DOE Contact L.K. Len, (301) 903-3233; DSP Alloys Contact Mr. Gordon G. Chase, (858) 274-9228

Development of Internal-Tin Nb/Sn Strand for High Field Accelerator Dipole Applications - DOE Contact L.K. Len, (301) 903-3233; Hyper Tech Research, Inc. Contact Mr. Michael Tomsic, (937) 332-0348

Engineered Ceramic Composite Insulators for High Field Magnet Applications - DOE Contact L.K. Len, (301) 903-3233; Multiphase Composites Contact Mr. John A. Rice, (303) 684-9242

FY 2004 PHASE II (SECOND YEAR)

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

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

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

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

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

Transformer Ratio Enhancement Experiment for Next Generation Dielectric Wakefield Accelerators - DOE Contact L.K. Len, (301) 903-3233; Euclid Concepts LLC Contact Dr. A.D. Kanereykin, (440) 519-0410

High Current Density (Jc), Low AC Loss, Low Cost Internal-Tin Superconductors - DOE Contact L.K. Len, (301) 903-3233; Supergenics Contact Mr. Bruce Zeitlin, (941) 349-0930

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

Micro-Photomultiplier Array - DOE Contact Blaine Norum, (301) 903-4398; Nanosciences Corporation Contact Dr. Charles Beetz, (203) 267-4440

Electrically Medicated Microetching Manufacturing Process to Replace Emersion and Spray Etching - DOE Contact Blaine Norum, (301) 903-4398; Faraday Technology, Inc. Contact Dr. E. Jennings Taylor, (937) 836-7749

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

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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2004 PHASE I

Innovative, Low Cost, Radiation-Resistant Fusion Magnet Insulation - DOE Contact Warren Marton, (301) 903-4936; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Development of a Canonical Approach to Liquid Metal MHD Computations and Experiments - DOE Contact Gene Nardella, (301) 903-4956; Hypercomp, Inc. Contact Dr. Vijaya Shankar, (818) 865-3713

Hybrid Spinel Composites: Unique Radiation Resistant Refractories - DOE Contact Madeline Feltus, (301) 903-2308; Technology Assessment and Transfer, Inc. Contact Mrs. Sharon Fehrenbacher, (301) 261-8373

Novel, High Energy Density Intermetallic Anode Material for Li-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Farasis Energy, Inc. Contact Dr. Keith D. Kepler, (510) 864-4800

Self-Cleaning Surfaces with Morphology Mimicking Superhydrophobic Biological Surfaces - DOE Contact Charles Russomanno, (202) 586-7543; Ngimat Co. Contact Dr. Andrew T. Hunt, (678) 287-2402

Investigation of $(CaO)_x(Al_2O_3)_x$ for Thermal Insulation and Molten Aluminum Contact - DOE Contact Sara Dillich, (202) 586-7925; Westmoreland Advanced Materials Contact Dr. Kenneth A. McGowan, (724) 339-2041

Use of Amended Silicates for Multi-Pollutant Control in Gasifiers - DOE Contact Jenny Tennant, (304) 285-4830; Ada Technologies, Inc. Contact Mr. Clifton H. Brown, Jr., (303) 792-5615

FY 2004 PHASE II (FIRST YEAR)

A Design of a New Readout Sensor for Spect - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

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

Electrodecontamination for Mitigation of Airborne Contamination - DOE Contact Justine Alchowiak, (202) 586-4629; Ada Technologies, Inc. Contact Mr. Clifton H. Brown, Jr., (303) 792-5615

Evaluation of a Novel Magnetic Activated Carbon Process for Gold Recovery - DOE Contact Michael Canty, (202) 586-8119; Eriez Manufacturing Contact Mr. Chester F. Giermak, (814) 835-6000

Tailorable, Environmental Barrier Coatings for Super-Alloy Turbine Components in Syngas - DOE Contact Udaya Rao, (412) 386-4743; Ceramatec, Inc. Contact Mr. Raymond K. Miller, (801) 978-2114

Hot Section Material Systems Testing and Development for Advanced Power Systems - DOE Contact Udaya Rao, (412) 386-4743; Florida Turbine Technologies, Inc. Contact Mrs. Shirley Coates Brostmeyer, (561) 746-3317

SiCN High Temperature Microelectromechanical Systems (MEMS) Sensor Suite - DOE Contact Susan Maley, (304) 285-1321; Sporian Microsystems, Inc. Contact Mr. Wenge Zhang, (303) 516-9075

Enhanced Performance Carbon Foam Heat Exchanger for Power Plant Cooling - DOE Contact Barbara Carney, (304) 285-4671; Ceramic Composites, Inc. Contact Mrs. Sharon Fehrenbacher, (410) 224-3710

Dehydration of Natural Gas - DOE Contact Tony Zammerilli, (304) 285-4641; Membrane Technology and Research, Inc. Contact Ms. Elizabeth Weiss, (650) 328-2228

High Pressure Economical Process for Treating Natural Gas - DOE Contact Tony Zammerilli, (304) 285-4641; TDA Research, Inc. Contact Mr. John D. Wright, (303) 940-2300

Novel Fischer-Tropsch Reactor - DOE Contact Kathy Stirling, (918) 699-2008; Ceramem Corporation Contact Dr. Robert L. Goldsmith, (781) 899-4495

Innovative Inorganic Fusion Magnet Insulation Systems - DOE Contact Warren Marton, (301) 903-4956; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Aluminum Nitride Radio Frequency Windows - DOE Contact Blaine Norum, (301) 903-4398; Sienna Technologies, Inc. Contact Dr. Ender Savrun, (425) 485-7272

A Novel Design for CZT Gamma Ray Spectrometers - DOE Contact Blaine Norum, (301) 903-4398; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Some Improved Methods of Introducing Additional Elements into Internal-tin Nb_3Sn - DOE Contact L.K. Len, (301) 903-3233; Supergenics, LLC Contact Mr. Bruce Zeitlin, (941) 349-0930

Fast X-Band Phase Shifter - DOE Contact L.K. Len, (301) 903-3233; Omega-P, Inc. Contact Dr. George P. Trahan, (203) 789-1164

Near Net Shape Manufacturing Using Combustion Driven Compaction - DOE Contact L.K. Len, (301) 903-3233; Utron, Inc. Contact Dr. F. Douglas Witherspoon, (703) 369-5552

FY 2004 PHASE II (SECOND YEAR)

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

Stabilized Lithium Manganese Oxide Spinel Cathode for High Power Li-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Farasis Energy, Inc. Contact Dr. Keith D. Kepler, (650) 594-4380

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2004 PHASE I

Lower Cost Nb_3Sn Internal-Tin Strand for ITER Fusion Project - DOE Contact Warren Marton, (301) 903-4936; Hyper Tech Research Inc Contact Mr. Michael Tomsic, (937) 332-0348

Flowing Liquid Lithium Walls Using Engineered Surfaces - DOE Contact Gene Nardella, (301) 903-4956; Plasma Processes, Inc. Contact Mr. Timothy N. McKechnie, (256) 851-7653

Ternary Nb-Ti-Ta Alloys for High Field 2 K Applications—Alloy Selection and Process Optimization - DOE Contact L.K. Len, (301) 903-3233; Global Research And Development, Inc. Contact Mr. Michael Tomsic, (937) 332-0348

High Superconductor Fraction, High Engineering Critical Current Density Bi-2212/Ag Wires Fabricated by Ultrasonic Wire Drawing - DOE Contact L.K. Len, (301) 903-3233; Global Research and Development, Inc. Contact Mr. Michael J. Tomsic, (937) 332-0348

Increase Piece Length and Reduce Cost of A15 Superconductor Wire by Eliminating Wire Drawing Breakage - DOE Contact L.K. Len, (301) 903-3233; Innovare, Inc. Contact Dr. Alfred R. Austen, (610) 837-8830

Moldable Ceramic Composites for High Field Magnet Applications - DOE Contact L.K. Len, (301) 903-3233; Multiphase Composites Contact Mr. John A. Rice, (303) 684-9396

Low Loss Ferroelectric Material Development for Accelerator Applications - DOE Contact L.K. Len, (301) 903-3233; Euclid Techlabs, LLC Contact Dr. A. D. Kanareykin, (440) 519-0410

Advanced Fluoropolymer Vessels for Ultra-Clean Ionization and Scintillation Detectors - DOE Contact Saul Gonzalez, (301) 903-2359; Applied Plastics Technology, Inc. Contact Mr. Andrew K. MacIntyre, (401) 253-0200

Coaxial Energetic Ion Depostition of Superconducting Coatings on Copper RF Cavities for Particle Accelerators - DOE Contact Blaine Norum, (301) 903-4398; Alameda Applied Sciences Corporation (AASC) Contact Dr. Mahadevan Krishnan, (510) 483-4156

A Method for Electroforming Copper with Ultra-Low Levels of Radioactivity - DOE Contact Blaine Norum, (301) 903-4398; Reeves & Sons, LLC Contact Mr. James H. Reeves, (509) 943-1653

Novel Micro-Nanoprobes and Detection Method for Biomedical Applications - DOE Contact Roland Hirsch, (301) 903-9009; Microcosm, Inc. Contact Dr. Wayne E. Moore, (301) 725-2775

Ceramic Composite Fuel Encapsulation in High Efficiency, Advanced Pebble-Bed Gas Reactors - DOE Contact Madeline Feltus, (301) 903-2308; Hyper-Therm High-Temperature Composites, Inc. Contact Mr. Wayne S. Steffier, (714) 375-4085

Anode Electrolyte Nanocomposites as Alternative to Carbonaceous Anode Materials - DOE Contact Jim Barnes, (202) 586-5657; nGimat Co. Contact Dr. Andrew Hunt, (678) 287-2402

Polythiophosphonate Electrolytes for Rechargeable Magnesium Batteries - DOE Contact Jim Barnes, (202) 586-5657; Phoenix Innovation Inc. Contact Mr. R. Scott Morris, (508) 291-4375

Lithium Ion-Channel Polymer Electrolyte for Lithium Metal Anode Rechargeable Batteries - DOE Contact Jim Barnes, (202) 586-5657; TDA Research, Inc. Contact Mr. John D. Wright, (303) 940-2300

Low Cost, High Performance PPSA-Based PEM Fuel Cell Membranes - DOE Contact Donna Ho, (202) 586-8000; T/J Technologies, Inc. Contact Mrs. Maria A. Thompson, (734) 213-1637

Oxidation Protection via Nanocrystalline Coatings - DOE Contact Charles Russomanno, (202) 586-7543; Material Interface, Inc. Contact Dr. Susan Kerber, (262) 246-9610

Shape Memory Polymer Nanocomposites - DOE Contact Charles Russomanno, (202) 586-7543; Nei Corporation Contact Dr. Ganesh Skandan, (732) 868-1906

Novel Nanoscale Intermetallic Fuel Cell Catalyst Materials and Processing - DOE Contact Charles Russomanno, (202) 586-7543; Primet Precision Materials, Inc. Contact Dr. Leonard E. Dolhert, (410) 531-6349

Novel, Active Layer Nanostructures for White Light Emitting Diodes (LEDS) - DOE Contact James Brodrick, (202) 586-1856; Dot Metrics Technologies Contact Ms. Rosanna Stokes, (704) 604-0653

High Efficiency Nanocomposite White Light Phosphors - DOE Contact James Brodrick, (202) 586-1856; Nanosys, Inc. Contact Ms. Karen Vergura, (650) 331-2114

New, Efficient Nanophase Materials for Blue and Deep Green Light-Emitting Diodes - DOE Contact James Brodrick, (202) 586-1856; Nomadics, Inc. Contact Mr. James H. Luby, (405) 372-9535

Composite Metal-Ceramic Hydrogen Separation Membranes - DOE Contact Charles Russomanno, (202) 586-7543; Synkera Technologies, Inc. Contact Dr. Stephen S. Williams, (720) 494-8401

High Temperature Pervaporation Membrane and Process - DOE Contact Charles Russomanno, (202) 586-7543; Trans Ionics Corporation Contact Dr. Robert C. Schucker, (281) 296-5585

Functionally Graded Aluminum Nitride - Oxide Coatings for Hot Pipe Protection - DOE Contact Sara Dillich, (202) 586-7925; Eltron Research, Inc. Contact Ms. Eileen E. Sammells, (303) 530-0263

Development of Solar Grade (SoG) Silicon - DOE Contact Alec Bulawka, (202) 586-5633; Crystal Systems, Inc. Contact Dr. Chandra P. Khattak, (978) 745-0088

An Innovative Technique of Preparing Solar Grade Silicon Wafers from Metallurgical Grade Silicon by In-Situ Purification - DOE Contact Alec Bulawka, (202) 586-5633; GT Equipment Technologies, Inc. Contact Mr. Jonathan A. Talbott, (603) 883-5200

Light-Weight Nanocrystalline Hydrogen Storage Materials - DOE Contact Richard J. Dunst, (412) 386-6694; Advanced Materials Corporation Contact Dr. S. G. Sankar, (412) 921-9600

FY 2004 PHASE II (FIRST YEAR)

Al(In)GaN-Based, High-Electron Mobility Transistors (HEMTs) on SiC for High-Power Radar Applications - DOE Contact Vaughn Standley, (202) 586-1874; SVT Associates Contact Ms. Janes Marks, (952) 934-2100

Cell-Free Protein Synthesis for High-Through-Put Proteomics - DOE Contact Marvin Stodolsky, (301) 903-4475; Macconnell Research Corporation Contact Dr. William P. MacConnell, (858) 452-2603

Low-Cost Automatic Tool Fixturing Based on Dexterous Robotic Hand - DOE Contact Justine Alchowiak, (202) 586-4629; Barrett Technology, Inc. Contact Mr. Burt Doo, (617) 252-9000

Solid-State Thermal-Neutron Detector Based on Boron-Doped a-Se Stabilized Alloy Films - DOE Contact Helen Kerch, (301) 903-2346; EIC Laboratories, Inc. Contact Dr. R. David Rauh, (781) 769-9450

New, Stable Cathode Materials for OLEDs - DOE Contact Ryan Egidi, (304) 285-0945; International Technology Exchange, Inc. Contact Dr. Terje Skotheim, (520) 299-9533

Novel Lower-Voltage OLEDs for Higher-Efficiency Lighting - DOE Contact James Brodrick, (202) 586-1856; Universal Display Corporation Contact Ms. Janice K. Mahon, (609) 671-0980

$LiFePO_4$ Cathode Material Designed for Use in Lithium-Ion Batteries with Application to Electric and Hybrid-Electric Vehicles - DOE Contact Jim Barnes, (202) 586-5657; Tiax, LLC Contact Ms. Renee Wong, (617) 498-5655

Metal Oxide Catalyst for Methyl Ethyl Ketone Production via One-Step Oxidation of n-Butane - DOE Contact Charles Russomanno, (202) 586-7543; Evernu Technology, LLC Contact Dr. Manhua Mandy Lin, (215) 659-8574

Low Cost and High Performance, Polymer Nanocomposite, Specialty Industrial Coatings - DOE Contact Charles Russomanno, (202) 586-7543; NEI Corporation Contact Dr. Gary Tompa, (732) 885-1088

Industrial Nano Material Components with High Temperature Corrosion and Wear Resistance Performance for Energy Savings - DOE Contact Brian Valentine, (202) 586-1739; IAP Research, Inc. Contact Dr. John P. Barber, (937) 296-1806

High Temperature-Stable Membrane Electrode Assemblies for Fuel Cells Fabricated via Ink Jet Deposition - DOE Contact Brian Valentine, (202) 586-1739; Nanosonic, Inc. Contact Dr. Richard O. Claus, (540) 953-1785

Cost Effective Improved Refractory Materials for Gasification Systems - DOE Contact Jenny Tennant, (304) 285-4830; Blasch Precision Ceramics, Inc. Contact Mr. John R. Parrish, (518) 436-1263

Advanced Net-Shape Insulation for Solid Oxide Fuel Cells - DOE Contact Travis Shultz, (304) 285-1370; Ceramatec, Inc. Contact Mr. Raymond K. Miller, (801) 978-2144

High-Performance, Plasticization-Resistant Membranes for Natural Gas Separations - DOE Contact Tony Zammerilli, (304) 285-4641; Membrane Technology and Research, Inc. Contact Ms. Elizabeth Weiss, (650) 328-2228

Cost Effective Fischer-Tropsch Technology - DOE Contact Kathy Stirling, (918) 699-2008; Exelus, Inc. Contact Mr. Mitrajit Mukherjee, (973) 740-2350

Nanocomposite Dielectric Materials for High Frequency Applications - DOE Contact T. V. George, (301) 903-4957; TPL, Inc. Contact Mr. Harold M. Stoller, (505) 342-4412

Very Large, High Gain APDs for Particle Physics - DOE Contact Saul Gonzalez, (301) 903-2359; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

FY 2004 PHASE II (SECOND YEAR)

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

Catalyst to Improve Small-Scale Claus Plants - DOE Contact Tony Zammerilli, (304) 285-4641; TDA Research, Inc. Contact Mr. John D. Wright, (303) 940-2300

LSGM Based Composite Cathodes for Anode Supported, Intermediate Temperature (600-800 degrees C) Solid Oxide Fuel Cells (SOFC) - DOE Contact Lane Wilson, (304) 285-1336; Materials and Systems Research, Inc. Contact Dr. Dinesh K. Shetty, (801) 530-4987

Metal Oxide Catalyst for Methacrylic Acid Preparation via One-Step Oxidation of Isobutane - DOE Contact Charles Russomanno, (202) 586-7543; Evernu Technology, LLC Contact Dr. Manhua Mandy Lin Ph.D, (215) 649-8574

P-Type ZnO Films - DOE Contact Satyen Deb, (303) 384-6405; Structured Materials Industries, Inc. Contact Dr. Gary S. Tompa, (732) 885-5909

An Advanced Cathode Material for Li-Ion Battteries - DOE Contact Jim Barnes, (202) 586-5657; A123 Systems Contact Mr.Ric Fulop, (617) 250-0565

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

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

Growth of a New, Fast Scintillator Crystal for Nuclear Experiments - DOE Contact Blaine Norum, (301) 903-4398; Ceramare Corporation Contact Dr. Larry E. McCandlish, (732) 937-8260

A New Scintillator for Gamma Ray Spectroscopy - DOE Contact Blaine Norum, (301) 903-4398; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Diamond Windows for High Power Microwave Transmission - DOE Contact T. V. George, (301) 903-4957; Coating Technology Solutions, Inc. Contact Dr. Roy Gat, (617) 625-2725

Radiation Resistant Insulation with Improved Shear Strength for Fusion Magnets - DOE Contact Warren Marton, (301) 903-4958; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Nanostructured Tungsten for Improved Plasma Facing Component Performance - DOE Contact Gene Nardella, (301) 903-4956; Plasma Processes, Inc. Contact Mr. Timothy McKechnie, (256) 851-7653

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

High Resolution Gamma Ray Spectrometer for Nuclear Non-Proliferation - DOE Contact Frances Keel, (202) 586-2197; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 926-1167

Growth of a New Mid-IR Laser Crystal - DOE Contact Frances Keel, (202) 586-2197; Ceramare Corporation Contact Dr. Larry E. McCandlish, (732) 937-8260

Induim Arsenide Antimonide Very Long Wavelength Photodiodes for Near Room Temperature Operation - DOE Contact Frances Keel, (202) 586-2197; SVT Associates Contact Ms. Jane Marks, (952) 934-2100

INSTRUMENTATION AND FACILITIES

FY 2004 PHASE I

Novel Scintillator for Nuclear Physics Studies - DOE Contact Blaine Norum, (301)903-4398; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617)668-6800

Ultra-Low Background Alpha Activity Counter - DOE Contact Blaine Norum, (301)903-4398; XIA, LLC Contact Dr. William K. Warburton, (510)494-9020

Ultra-Sensitive, Compact Mid-Infrared Spectrometer for Airborne and Ground-Based Atmospheric Monitoring - DOE Contact Rick Petty, (301) 903-5548; Novawave Technologies, Inc. Contact Dr. James Scherer, (650) 610-0956

FY 2004 PHASE II (FIRST YEAR)

Situational Awareness Monitor for Nuclear Events - DOE Contact Frances Keel, (202) 586-2187; ADA Technologies, Inc. Contact Mr. Clifford H. Brown, Jr., (303) 792-5615

Low-Noise Borehole Triaxial Seismometer - DOE Contact Frances Keel, (202) 586-2197; Geotech Instruments, LLC Contact Dr. Lani Oncescu, (214) 221-0000

Compact, Short-Pulse Laser Source for Active Imaging Systems - DOE Contact Frances Keel, (202) 586-2197; Aculight Corporation Contact Dr. Dennis Lowenthal, (425) 482-1100

Advanced, Aerosol Mass Spectrometer for Aircraft Measurement of Organic Particulate Matter - DOE Contact Michael Huesemann, (360) 681-3618; Aerodyne Research, Inc. Contact Dr. Charles E. Kolb, (978) 663-9500

Cavity Attenuation Phase Shift Spectroscopic Detection of Nitrogen Dioxide - DOE Contact Michael Huesemann, (360) 681-3618; Aerodyne Research, Inc. Contact Dr. Charles E. Kolb, (978) 663-9500

Novel Ultrasensitive Instrumentation for Trace Gas Measurements in the Field - DOE Contact Michael Huesemann, (360) 681-3618; Los Gatos Research Contact Ms. Noel Wong O'Keefe, (650) 965-7780

Innovative Carbon Dioxide Sensor Based on Cavity Ringdown - DOE Contact Roger Dahlman, (301) 903-4951; Picarro, Inc. Contact Mr. Tom Oswold, (408) 470-6099

High Precision CO_2 Sensor for Balloon Sonde Atmospheric Measurements - DOE Contact Roger Dahlman, (301) 903-4951; Southwest Sciences, Inc. Contact Dr. Alan C. Stanton, (505) 984-1322

A Down-Hole Probe for Real-Time Ore Grade Assessment in "Look Ahead" Mining - DOE Contact Michael Canty, (202) 586-8119; Resonon, Inc. Contact Dr. Michael R. Kehoe, (406) 586-3356

Development of HSTAT for HVAC Health Status and Control - DOE Contact Terrence Logee, (202) 586-1689; Steven Winter Associates, Inc. Contact Mr. Steven Winter, (203) 857-0200

An Extremely High Power, Field-Coupled, Low-Loss RF Transmission Line for SRF Cavities - DOE Contact Blaine Norum, (301) 903-4398; AVAR, Inc. Contact Ms. Roisin Preble, (757) 595-4643

Magnetized Electron Transport in the Proposed Electron Cooling Section of the Relativistic Heavy Ion Collider - DOE Contact Blaine Norum, (301) 903-4398; Tech-X Corporation Contact Dr. John R. Cary, (303) 448-0727

Ultra High Speed Analog to Digital Converter with Ternary Digital Output - DOE Contact Blaine Norum, (301) 903-4398; Advanced Science and Novel Technology Company Contact Dr. Vladimir Katzman, (310) 377-6029

High Precision, Integrated Beam Position and Emittance Monitor - DOE Contact L.K. Len, (301) 903-3233; Far-tech, Inc. Contact Mr. Jin-Soo Kim, (858) 455-6655

Six-Dimensional Beam Cooling in a Gas Absorber - DOE Contact L.K. Len, (301) 903-3233; Muons, Inc. Contact Ms. Linda L. Even, (757) 930-1463

High-Power Radio Frequency Window - DOE Contact L.K. Len, (301) 903-3233; Asgard Microwave Contact Mr. David B. Aster, (509) 534-5011

Hybrid Modulator Upgrade - DOE Contact L.K. Len, (301) 903-3233; Diversified Technologies, Inc. Contact Mr. Michael A. Kempkes, (781) 275-9444

NLC Marx Bank Modulator - DOE Contact L.K. Len, (301) 903-3233; Diversified Technologies, Inc. Contact Mr. Michael A. Kempkes, (781) 275-9444

Quasi-Optical 34-GHz Radio Frequency (RF) Pulse Compressor - DOE Contact L.K. Len, (301) 903-3233; Omega-P, Inc. Contact Dr. George P. Trahan, (203) 789-1164

A Hydrostatic Processing Facility for Superconducting Wire - DOE Contact L.K. Len, (301) 903-3233; Alabama Cryogenic Engineering, Inc. Contact Ms. Mary T. Hendricks, (256) 536-8629

Novel Magnetometer for Quadrupole and Dipole Magnetic Measurements - DOE Contact L.K. Len, (301) 903-3233; Tai-Yang Research Corporation Contact Dr. Christopher M. Rey, (302) 494-4048

FY 2004 PHASE II (SECOND FIRST YEAR)

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

High Gain, Fast Scan, Broad Spectrum, Parallel Beam Wavelength Dispersive X-Ray Spectrometer for SEM - DOE Contact Dean Miller, (630) 252-4108; Parallax Research, Inc. Contact Mr. David Ohara, (850) 580-5481

Advanced X-Ray Detectors for Transmission Electron Microscopy - DOE Contact Dean Miller, (630) 252-4108; Photon Imaging, Inc. Contact Dr. Bradley E. Patt, (818) 709-2468

Using Convergent Beams for Small-Sample, Time-of-Flight Neutron Diffraction - DOE Contact Helen Kerch, (301) 903-2346; X-Ray Optical Systems, Inc. Contact Mr. David Usher, (518) 464-3334

MATERIALS STRUCTURE AND COMPOSITION

FY 2004 PHASE I

Microstructural Refinement of Tantalum for Superconductor Diffusion Barrier Applications - DOE Contact L.K. Len, (301) 903-3233; Shear Form, Inc. Contact Dr. K. T. Hartwig, (979) 693-4102

"Metal Rubber" Nanostructured Materials - DOE Contact Charles Russomanno, (202) 586-7543; Nanosonic, Inc. Contact Dr. Richard O. Claus, (540) 953-1785

High Extraction Luminescent Material Structures for Solid State Light Emitting Diodes - DOE Contact James Brodrick, (202) 586-1856; Phosphortech Corporation Contact Dr. Hisham M. Menkara, (404) 664-5008

FY 2004 PHASE II (SECOND YEAR)

Development of a New, Low Frequency, Rf-Focused Linac Structure - DOE Contact Blaine Norum, (301) 903-4398; Linac Systems Contact Mrs. Barbara C. Swenson, (505) 798-1904

SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2004 PHASE I

Solid state and Resistance Joining Technologies for Fusion Energy Systems – DOE Contact Gene Nardella, (301) 903-4171; DDL OMNI Engineering, LLC Contact Mr. Charles Zanis, (703) 918-4320

Advanced Plasma Gun Development for Simulating Edge-Localized-Mode Plasma Disruptions with Application to Free Surface Flowing Liquid Metal PFCs – DOE Contact Gene Nardella, (301) 903-4171; Starfire Industries LLC Contact Dr. Robert A. Stubbers, (217) 390-2784

Thinner Silicon Detectors and Novel Interconnections for Robust High Energy Physics Detectors - DOE Contact Saul Gonzalez, (301) 903-2890; Digital Optics Corporation Contact Dr. Rich Jones, (704) 887-3130

Ultra-Trace Molecular Detection Instrumentation Based on Aerosol Nucleation with Rapid Preconcentration and Separation – DOE Contact Stephen Chase, (202) 586-3789; InnovaTek, Inc. Contact Dr. Vladimir B. Mikheev, (509) 375-1093

Novel Photocatalytic Energy Converter for Nuclear Safeguards Applications – DOE Contact Stephen Chase, (202) 586-3789; Konarka Technologies, Inc. Contact Dr. Russell Gaudiana, (978) 569-1410

A Compact, In-Situ Instrument for Organic Acids – DOE Contact Rick Petty, (301) 903-5548; Aerosol Dynamics, Inc. Contact Dr. Susanne Hering, (510) 649-9360

Efficient Nanotube-Based OLEDs – DOE Contact James Brodrick, (202) 586-1856; NanoTex Corporation Contact Dr. L.P. Felipe Chibante, (713) 777-6266

FY 2004 PHASE II (FIRST YEAR)

Engineered Tungsten Surfaces for IFE Dry Chamber Walls - DOE Contact Gene Nardella, (301) 903-4956; Plasma Processes, Inc. Contact Mr. Timothy McKechnie, (856) 851-7653

FY 2004PHASE II (SECOND YEAR)

Carbon Fiber Composite Aeroelastically Tailored Rotor Blades for Utility-Scale Wind Turbines - DOE Contact John Cadogan, (202) 586-1991; K. Wetzel & Company Contact Dr. Kyle K. Wetzel, (785) 766-2450

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2004 PHASE II (SECOND YEAR)

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2004 PHASE I

Fabrication of Chemically Doped, High Upper Critical Field Magnesium Diboride Superconducting Wires - DOE Contact Warren Marton, (301) 903-4936; Speciality Materials, Inc. Contact Dr. Ray Suplinskas, (978) 322-1977

Nanocomposite Membranes for High Temperature Proton Exchange Membrane Fuel Cells – DOE Contact Donna Ho, (202) 586-8000; Pacific Fuel Cell Corporation Contact Mr. George Suzuki, (714) 564-1693

Polymer Composite Barrier System for Encapsulating LEDs – DOE Contact James Brodrick, (202) 586-1856; T/J Technologies, Inc. Contact Dr. Suresh Mani, (734) 213-1637

Surface Modification of Nanoporous Zeolite Pervaporation Membranes for Enhanced Biomass Product Recovery - DOE Contact Charles Russomanno, (202) 586-7543; ITN Energy Systems, Inc. Contact Dr. Brian S. Berland, (303) 285-5107

Bulk Nanophase High Transition Temperature Shape Memory Alloys for Novel Waste Heat Recovery Systems - DOE Contact Sara Dillich, (202) 586-7925; Material & Electrochemical Research (MER) Corporation Contact Dr. Sion Pickard, (520) 574-1980

Conformal Power Harvesting Microstructures – DOE Contact Gideon Varga, (202) 586-0082; Materials and Power Technologies, LLC Contact Dr. Mathias Hecht, (520) 370-7564

FY 2004 PHASE II (FIRST YEAR)

Nanostructured Polymeric Heterogeneous Catalyst for Industrial Applications - DOE Contact Charles Russomanno, (202) 586-7543; TDA Research, Inc. Contact Mr. John Wright, (303) 940-2300

Novel Approach Toward High Performance Energetic Rays Detection - DOE Contact Jehanne Simon-Gillo, (301) 903-1455; Lutronics Inc. Contact Dr. Yalin Lu, (978) 387-9685

FY 2004 PHASE II (SECOND YEAR)

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

INSTRUMENTATION AND FACILITIES

FY 2004PHASE I

High Brightness Neutron Source for Radiography – DOE Contact Madeline Feltus, (301) 903-2308; Adephi Technology, Inc. Contact Dr. Jay Theodore Cremer, (650) 598-9800

OFFICE OF FUSION ENERGY SCIENCES

The mission of the Office of Fusion Energy Sciences (OFES) is to advance plasma science, fusion science, and fusion technology—the knowledge base needed for an economically and environmentally- attractive fusion energy source. Fusion materials research is a key element of the longer-term OFES mission, focusing on the effects on materials properties and performance from exposure to the radiation, energetic particle, thermal, and chemical environments anticipated in the chambers of fusion experiments and energy systems. The unique requirements on materials for fusion applications are dominated by the intense energetic neutron environment characteristic of the deuterium-tritium fusion reaction. Materials in the fusion chamber must have slow and predictable degradation of properties in this neutron environment. For safety and environmental considerations, "low activation" materials must be selected with activation products that neither decay too rapidly(affecting such safety factors as system decay heat) nor too slowly (affecting the waste management concerns for end-of-life system components).Structural materials research focuses on issues of microstructural stability, fracture and deformation mechanics, and the evolution of physical and mechanical properties. This research provides a link between fusion and other materials science communities and contributes in niche areas toward grand challenges in general fields of materials science. Growth in the theory, modeling, and simulation elements of this research are providing for leveraging of advances in nano-technology and computational materials science research. Non-structural materials research focuses on plasma facing materials that protect structural materials from intense heat and particle fluxes and extract surface heat deposited by plasmas without rapid deterioration and or emitting levels of impurities that could degrade plasma performance. Fusion materials research is conducted with a high degree of international cooperation. Bilateral agreements with Japan enhance the ability of each party to mount fission reactor irradiation experiments. Agreements under the International Energy Agency provides for the exchange of information and the coordination of fusion materials programs in the US, Japan, Europe, Russia, and China. The DOE Contact is G. Nardella, 301-903-4956.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

181. VANADIUM ALLOY AND INSULATING COATING RESEARCH
$1,500,000
DOE Contact: G. Nardella, 301-903-4956
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

182. THEORY AND MODELING
$1,700,000
DOE Contact: G. Nardella, 301-903-4956
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 their radiation 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 ©) 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

183. FERRITIC/MARTENSITIC STEEL RESEARCH
$2,300,000
DOE Contact: G. Nardella, 301-903-4956
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 than 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

184. SiC/SiC COMPOSITES RESEARCH
$1,500,000
DOE Contact: G. Nardella, 301-903-4956
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 ont he 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

185. PLASMA FACING MATERIALS RESEARCH
$2,000,000
DOE Contact: G. Nardella, 301-903-4956
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 minimize replacement frequency, and provide for reduced neutron activation to minimize decay heat and radioactive waste burdens. Research activities include improved techniques for joining beryllium or tungsten to copper alloys, development of joining techniques for refractory metals (e.g., W, Mo, Nb, V),development of enhancement schemes for helium cooling or liquid lithium cooling of refractory alloys, and thermal fatigue testing of tungsten and other refractory materials.The joining techniques being investigated include diffusion bonding, hot-isostatic pressing, furnace brazing and inertial welding. Tritium retention and permeation measurements are conducted in the Tritium Plasma Experiment and the PISCES plasma simulator facility. Refractory material work is centered on developing high temperature helium gas cooled or liquid metal cooled heat sinks for plasma facing components. The thermal fatigue testing and heat removal capability measurements are carried out on electron beam test systems.

Keywords: Plasma-Facing Materials, Refractory Metals

OFFICE OF BIOLOGICAL & ENVIRONMENTAL RESEARCH

The Biological and Environmental Research (BER) program develops the knowledge needed to identify, understand, anticipate, and mitigate the long-term health and environmental consequences of energy production, development, and use. As the founder of the Human Genome Project, BER continues to play a major role in biotechnology research and also invests in basic research on global climate change and environmental remediation.

The projects listed in this report are managed under the Environmental Management Research Program (EMSP). Basic research under the EMSP contributes to environmental management activities that decrease risk to the public and workers, provide opportunities for major cost reductions, reduce time required to achieve the

Department's environmental management goals, and, in general, address problems that are considered intractable without new knowledge. The entire EMSP portfolio can be viewed on the World Wide Web by accessing the EMSP home page at http://emsp.em.doe.gov. The EMSP program was transferred to the Office of Science in FY 2003. The current EMSP Director is Roland F. Hirsch, 301-903-9009.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

186. IRON PHOSPHATE GLASSES: AN ALTERNATIVE FOR VITRIFYING CERTAIN NUCLEAR WASTES
$79,000
DOE Contact: Roland F. Hirsch, 301-903-9009
University of Missouri-Rolla Contact:
Delbert E. Day, 573-341-4354

Borosilicate glass is the only material currently approved and being used to vitrify high level nuclear waste. Unfortunately, many high level nuclear waste feeds in the U.S. contain components which are chemically incompatible with borosilicate glasses. Current plans call for vitrifying even these problematic waste feeds in borosilicate glasses after the original waste feed has been pre-processed and/or diluted to compensate for the incompatibility. However, these pre-treatment processes, as well as the larger waste volumes resulting from dilution, will add billions of dollars to the DOE's cost of cleaning up the former nuclear weapons production facilities. Such additional costs may be avoided by developing a small number of alternative waste glasses which are suitable for vitrifying those specific waste feeds that are incompatible with borosilicate glasses.

A low cost and technically effective alternative waste form based on a new family of iron-phosphate glasses which appear to be well suited for many waste feeds, especially those which are incompatible with borosilicate glasses, has recently been developed. However, the scientific and technical knowledge base that is needed to vitrify nuclear waste in iron phosphate glasses on a production scale is currently lacking. In addition, the high priority wastes that are likely to cause problems in borosilicate melts need to be identified and property data need to be acquired for iron phosphate waste forms 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 suited for borosilicate glasses.

Keywords: Iron Phosphate Glasses, Vitrification, Nuclear Waste

187. PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW
$50,000
DOE Contact: Roland F. Hirsch, 301-903-9009
Pennsylvania State University Contact:
Michael Grutzeck, 814-863-2779
Savannah River Technology Center Contact:
Carol M. Jantzen, 803-725-2374

Natural and synthetic zeolites are extremely versatile materials. They can adsorb a variety of liquids and gases, and also take part in cation exchange reactions. Zeolites are easy to make, they can be synthesized from a wide variety of natural and man made materials. One such combination is metakaolinite and sodium hydroxide solution. The objective of this research is to adapt this well known reaction for use in site remediation and clean-up of caustic waste solutions now in storage in tanks at Hanford and the Savannah River sites.

It has been established that a mixture of calcined equivalent ICPP waste (sodium aluminate/hydroxide solution containing 3:1 Na:Al) and fly ash and/or metakaolinite can be cured at various temperatures to produce a monolith containing Zeolite A (80˚C) or Na-P1 plus hydroxysodalite (130˚C) dispersed in an alkali aluminosilicate hydrate matrix. The zeolitization process is a simple one and as such could be a viable alternative for fixation of low activity waste (LAW) salts and calcines. Dissolution tests have shown these materials to have superior retention for alkali, alkaline earth and heavy metal ions.

The technology for synthesizing zeolites is well documented for pure starting materials, but relatively little is known about the process if metakaolinite is mixed with a complex mixture of oxides containing nearly every element in the periodic table. The purpose of the proposed work is to develop a clearer understanding of the advantages and limitations of producing a zeolite-containing waste form from calcined radioactive waste, i.e., the effect of processing variables, reaction kinetics, crystal and phase chemistry, and microstructure on their performance. To accomplish this, two waste forms representative of solutions in storage at the Hanford and Savannah River sites will be simulated. Because nitrate is detrimental to the process, the LAW will be calcined at various temperatures (w/wo sugar) to maximize the reactivity of the resultant mix of oxide phases while minimizing the loss of volatiles. The oxides will be mixed with varying amounts and types of metakaolinite, small amounts of other chemicals (alkali hydroxides and/or carbonates, zeolite seeds, templating agents) and enough water to make a paste. The paste will then be cured (in-can) at a variety of temperatures (80°-100°C). Once reaction rates for the process are established, MAS NMR and TEM will be used to study the atomic-level structure of the solids. X-ray diffraction will be used to examine the degree of crystallinity of the waste forms. An environmental SEM will be used to track the development of microstructure in real time. An electron microprobe will be used to analyze the phases in the waste form. Attempts will be made to relate changes in phase chemistry and microstructure to distribution coefficients and dissolution data. Compressive and bending strength tests will be used to determine mechanical behavior and standard leach tests will be used to determine the potential consequences of cation exchange reactions. Since simulated waste is not an adequate predictor, a major portion of the proposed work will be carried out at the Savannah River Technology Center, using actual LAW samples obtained from the Savannah River site.

Keywords: Zeolites, Radioactive Waste

188. INVESTIGATING ULTRASONIC DIFFRACTION GRATING SPECTROSCOPY AND REFLECTION TECHNIQUES FOR CHARACTERIZING SLURRY PROPERTIES
$170,000
DOE Contact: Roland F. Hirsch, 301-903-9009
Pacific Northwest National Laboratory Contact:
Margaret S. Greenwood, 509-375-6801
University of Washington Contact:
Lloyd W. Burgess, 206-543-0579

The U.S. Department of Energy (DOE) has millions of gallons of radioactive liquid and sludge wastes that must be retrieved from underground storage tanks. This waste, in the form of slurries, must be transferred and processed to a final form, such as glass logs. On-line instrumentation to measure the properties of these slurries in real-time during transport is needed in order to prevent plugging and reduce excessive dilution. This project is a collaborative effort between Pacific Northwest National Laboratory (PNNL) and the University of Washington to develop a completely new method for using ultrasonics to measure the particle size and viscosity of a slurry. The concepts are based on work in optics on grating-light-reflection spectroscopy (GLRS) at the University of Washington and some preliminary work on ultrasonic diffraction grating spectroscopy (UDGS) that has already been carried out at PNNL. The project objective is to extend the GLRS theory for optics to ultrasonics, and to demonstrate its capabilities of UDGS. The viscosity of a slurry is measured by using the multiple reflections of a shear wave at the slurry-solid interface. This new ultrasonic method could result in an instrument that would be simple, rugged, and very small, allowing it to be implemented as part of a pipeline wall at facilities across the DOE complex.

Keywords: Diffraction Grating, Spectroscopy, Ultrasonic, Slurry, Viscosity, Particle Size

189. CHEMISTRY OF ACTINIDES IN MOLTEN GLASSES AND ITS CORRELATION TO STRUCTURAL PERFORMANCE OF SOLID GLASSES: FILLING THE KNOWLEDGE GAP
$140,000
DOE Contact: Roland F. Hirsch, 301-903-9009
Oak Ridge National Laboratory Contact:
Sheng Dai, 865-576-7307
Savannah River Technology Center Contact:
Ray F. Schumacher, 803-725-5991

Chemical processes occurring in molten glasses are key elements in determining efficient immobilization and the long term stability of glasses. The underlying goal of this research is to make use of high-temperature spectroscopic techniques to increase our fundamental understanding of the vitrification process, specifically the relationship between the chemistry of molten glasses and the structural features of final solid glasses. The fundamental knowledge gained in this study will fill a crucial knowledge gap concerning chemistry of actinides in molten glasses and have a broad impact on the design and construction of advanced vitrification processes. High temperature UV/Visible and near-IR spectral data will be used to investigate the solubility of actinide species in various molten glasses as a function of the composition and temperature. These data will be used to develop a new "optical basicity" scale for actinide stability and speciation in oxide glasses in analogy to the common pH scale used to define the acid-base properties of aqueous systems. Fluorescence lifetime distribution methods, fluorescence line-narrowing spectroscopy and X-ray absorption spectroscopy (XAS) will provide information on the local environment of the actinides while EPR and X-ray absorption edge positions will be used to define the oxidation states of actinide species in glasses. The combination of the optical basicity scale and structural information from fluorescence and XAS investigations, will be used to produce a detailed description of the identities and behavior of actinide species in silicate-based glasses. This stability model will be correlated to actinide leaching behavior for a glass matrix and offers a simple but powerful set of spectral "fingerprints" to predict the behavior of actinide species when immobilized in a glass.

Keywords: Molten Glasses, Spectroscopy, X-ray Absorption, Actinides

190. STABILITY OF HIGH LEVEL RADIOACTIVE WASTE FORMS
$290,000
DOE Contact: Roland F. Hirsch, 301-903-9009
Oak Ridge National Laboratory Contact:
Theodore M. Besmann, 865-574-6852
Pacific Northwest National Laboratory Contact:
John D. Vienna, 509-372-2807

High-level waste (HLW) glass compositions, processing schemes, limits on waste loading, and corrosion/dissolution release models are dependent on an accurate knowledge of liquidus temperatures and thermochemical values. Unfortunately, existing models for the liquidus are empirically-based, depending on extrapolations of experimental information. In addition, present models of leaching behavior of glass waste forms use simplistic assumptions of the thermochemistry or experimentally measured values obtained under non-realistic conditions. There is thus a critical need for both more accurate and more widely applicable models for HLW glass behavior. In a previous project significant progress was made in modeling HLW glass. Borosilicate glass was accurately represented along with the additional FeO-Fe_2O_3, Li_2O, K_2O, MgO, and CaO components. Nepheline precipitation, an issue in Hanford HLW formulations, was modeled and shown to be predictive. The objective of this effort is to continue the development of a basic understanding of the phase equilibria and solid solution of HLW glasses, incorporating other critical waste constituents including, S, Cr, F, P, actinides and rare earths. With regard to a fundamental understanding of solution oxides, there should be added insights on defect chemistry, interstitial behavior, clustering, and the energetics of metal oxide solutes.

Keywords: High-Level Waste, Glass, Phase Equilibria

191. 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 other chemicals. 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 radio analytical 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

192. 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 2004
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY - GRAND TOTAL	$13,130,000
OFFICE OF SPACE AND DEFENSE POWER SYSTEMS	$8,666,000
SPACE AND NATIONAL SECURITY PROGRAMS	$8,666,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$4,930,000
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	4,370,000
Carbon-Bonded Carbon Fiber Insulation Production, Maintenance, Manufacturing Process Development, and Product Characterization	560,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING	$3,736,000
Alloy Development Characterization, Mechanical Property Testing, and Insulation	1,447,000
Heat Source Fabrication Development and Materials Testing for IHS70 Program	2,289,000
OFFICE OF ADVANCED NUCLEAR RESEARCH	$4,464,000
ADVANCED FUEL CYCLE INITIATIVE	$2,464,000
Radiation Damage Modeling in AFCI Materials	224,000
Lead Alloy Technology	1,550,000
Structural Materials Testing	690,000
NUCLEAR HYDROGEN INITIATIVE	$2,000,000
Development of Advanced High-Temperature Heat Exchangers	2,000,000

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

193. 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
$4,370,000
DOE Contact: John Dowicki, 301-903-7729
ORNL Contacts: Jim King, 865-574-4807, Evan Ohriner, 865-574-8519, George Ulrich, 865-576-8497

The DOP-26 Iridium alloy is the fuel clad capsule material for radioisotope heat sources in NASA space power systems. The production capabilities and facilities for producing blank and foil stock material at ORNL was maintained by continuing all production activities to supply blanks and foil for clad vent set (CVS) production. The CVS production activity produces flight quality components for inventory and maintains the production capabilities for future production campaigns. The iridium inventory for DOE is maintained, audited, and reported annually.

During FY 2004, 160 flight quality iridium alloy blanks were produced and transferred to the CVS Production Task. Data packages were prepared for 61 pieces of iridium foil produced this year. Thirty-nine kilograms of iridium powder was purchased. One hundred-eighteen prime quality CVSs (44 of these were long cups for a heat source program) and seven “engineering use” CVSs were produced in FY 2004. The Annual Iridium Inventory Report was issued.

Keywords: Iridium Processing, Melting, Extrusion, Clad Vent Sets

194. CARBON-BONDED CARBON FIBER INSULATION PRODUCTION, MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT, AND PRODUCT CHARACTERIZATION
$560,000
DOE Contact: John Dowicki, 301-903-7729
ORNL Contacts: Jim King, 865-574-4807, Glenn Romanoski, 865-574-4838

The CBCF production facilities have been operated in a production maintenance mode since the Cassini campaign to produce flight quality insulators sets. Dedicated facilities for the CBCF production remain in the Carbon Materials Technology Laboratory at ORNL. Thirty-five prime quality CBCF insulator sleeves produced in FY 2002 and FY 2003 with impurity levels above the specification limit were dispositioned for engineering use. These sleeves meet all other property requirements. An additional 614 pounds of chopped rayon fiber was produced for production and certified for production use. A total of 16 additional prime quality CBCF sleeves and 60 discs were produced. Significant participation and leadership was provided to the GPHS Aeroshell Materials Working Group to determine a future path for obtaining Fine-Weaved Pierced Fabric material.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING

195. ALLOY DEVELOPMENT CHARACTERIZATION, MECHANICAL PROPERTY TESTING, AND INSULATION
$1,447,000
DOE Contact: John Dowicki, 301-903-7729
ORNL Contact: Jim King, 865-574-4807, Easo George, 865-574-5085, Robert Swindeman, 865-574-5108, James Hemrick, 865-574-7601

The activity provides the materials characterization, mechanical property information, and assessment of material behavior in specific applications to support various RPS Program needs. The characterization of iridium alloy DOP-26 has identified the effect of various impurities on the alloy properties and its manufacturing and service reliability. An alternate iridium alloy (DOP-40) containing less thorium and the addition of cerium has been developed and shown to have desirable properties. Mechanical property determinations are made on various alloys after thermal aging to assess their suitability for long-term terrestrial and space missions.

Significant progress was made in several areas during FY 2004. Testing was performed and a report on the low temperature impact properties of DOP-26 iridium alloy was issued. Testing was also performed to determine the influence of oxygen on the tensile properties of Ta-10W alloy over a range of temperatures.

Capsule pressure-burst and coupon creep rupture testing were performed on Haynes 25 alloy for a heat source program. This testing has continued successfully and periodic reports of the results were distributed. An investigation of the compatibility of Haynes 25 with graphite in a simulated generator environment was continued.

Test equipment was assembled and testing was performed to characterize the thermomechanical properties of Min-K 1400TE material. Testing was performed to determine the high temperature compressive strength and stress relaxation behavior of the material exposed to isothermal conditions and a under a thermal gradient.

Keywords: Iridium Alloy, Compatibility, Thermal Aging, Min-k Insulation

196. HEAT SOURCE FABRICATION DEVELOPMENT AND MATERIALS TESTING FOR IHS70 PROGRAM
$2,289,000
DOE Contact: John Dowicki, 301-903-7729
ORNL Contact: Jim King, 865-574-4807,
Mike Pershing, 865-576-4294

A radioisotope power system generator is being developed which utilizes iridium clad fuel enclosed in capsules of Ta-10W alloy, molybdenum, and Haynes 230. The Ta-10W capsule is designed to retain helium pressure during the service life. The outer capsule of Haynes 230 protects the refractory alloy from oxidation. ORNL is responsible for producing these capsule components for the new heat source. The iridium capsules are longer than the standard clad vent set to accommodate a larger fuel pellet. ORNL is conducting testing to produce a mechanical property data base to support the materials selection and design requirements.

Forty-four long iridium alloy CVSs were fabricated and shipped to LANL. Fabrication development activities continued for the various heat source components. A large heat of Ta-10W alloy material was purchased. Haynes 230 alloy and molybdenum was also purchased. Forming dies and fixtures were designed and fabricated for this project. Forming development was performed for the Ta alloy, Haynes alloy, and molybdenum components. Strength member capsules and clad bodies were produced for welding development. Refurbishment of ultra-high vacuum creep machines continued and capsule pressure burst machines were assembled. Creep testing of Ta-10W specimens was initiated.

Keywords: Ta-10W Fabrication, Refractory Metals, Mechanical Properties

OFFICE OF ADVANCED NUCLEAR RESEARCH

ADVANCED FUEL CYCLE INITIATIVE

The mission of the Advanced Fuel Cycle Initiative (AFCI) is to develop proliferation-resistant spent nuclear fuel treatment and transmutation technologies in order to enable a transition from the current once through nuclear fuel cycle to a future sustainable, closed nuclear fuel cycle. The intermediate-term issues associated with spent nuclear fuel, primarily the reduction of the volume and heat generation of material requiring geologic disposal, will be addressed using advanced separations technologies and proliferation-resistant recycle fuels in existing and advanced light water reactors, and possibly gas-cooled reactors if deployed in the near future. A longer-term effort will develop fuel cycle technologies to destroy minor actinides in fast neutron spectrum systems, greatly reducing the long-term radiotoxicity and heat load of high-level waste sent to a geologic repository. This will be accomplished through the development of a transmutation fuel cycle using Generation IV fast reactors.

197. RADIATION DAMAGE MODELING IN AFCI MATERIALS
$224,000
DOE Contact: Sue Lesica, 301-903-8755
LANL Contact: Mike Cappiello, 505-665-6408

Through the modeling of the mechanisms of radiation-induced helium production in body centered cubic iron, this research examines the loss of ductility as a function of helium production and displacements per atom (dpa). Also included is the identification of parameters to be experimentally measured to quantify the predictive model, methods to quantify these parameters experimentally and the proposal of experiments.

Keywords: Modeling, Ferritic Steel, Helium Embrittlement

198. LEAD ALLOY TECHNOLOGY
$1,550,000
DOE Contact: Sue Lesica, 301-903-8755
LANL Contact: Mike Cappiello, 505-665-6408

Coolant technology is focused on the development of lead-alloy heat-transport system materials and components. The Development of Lead-alloys

Technologies and Applications (DELTA) lead-bismuth test loop at LANL is the primary facility for this research. The loop is being used to perform corrosion, erosion, compatibility, thermal hydraulic, thermodynamic, radiation environment effects and instrumentation tests, with the support of off-line development of sensors, control systems, measurement and impurity removal techniques, and modeling. In addition to U.S. research, the facility is being used for international collaborations investigating lead coolant technologies. Long-term corrosion tests will be performed to systematically assess the performance of materials during the initial stage of oxide formation. Testing and analysis of specimens, component performance over time and under varying conditions, and lifetime limits will be determined. Development and testing of materials with enhanced corrosion resistance through special alloying and surface treatment will take place concurrently. Materials will be screened and assessed for high temperatures and coolant technology needs beyond oxygen control. Heat transfer and thermal hydraulic tests for reactor (e.g., fuel assembly to coolant heat transfer) and spallation target designs will be planned and performed. For the candidate fuel options, compatibility of coolant with fuel cladding and fuels will be investigated. The effects of radiation on corrosion, activation of corrosion products and mitigation strategies, radiation and spallation product influence on coolant chemistry and mitigation strategies will be studied. These effects will first be studied with surrogates and in simulated environments, and later in integral irradiation campaigns.

Keywords: Lead Bismuth, Transmutation

199. STRUCTURAL MATERIALS TESTING
$690,000
DOE Contact: Sue Lesica, 301-903-8755
LANL Contact: Mike Cappiello, 505-665-6408

The objective is to qualify structural materials of interest in a high-flux and high-fluence irradiation environment with high-energy particles relevant to fast-spectrum transmutation. This research examines the effect of high energy proton and neutron radiation on the mechanical properties of structural and target materials that could be used in an accelerator driven transmutation system.

Keywords: Transmutation, Irradiation, Structural Materials

NUCLEAR HYDROGEN INITIATIVE

The President's Hydrogen Fuel Initiative is a new research and development effort to reverse America's growing dependence on foreign oil and expand the availability of clean, abundant energy. Hydrogen is produced today on an industrial scale in the petrochemical industry by a process of steam reforming, using natural gas as both source material and heat source. The Department is exploring several processes for using heat and electricity from advanced high-temperature nuclear reactors to produce hydrogen. Nuclear heat, supplied to a hydrogen-producing thermochemical or electrolysis plant through an intermediate heat exchanger, promises high efficiency and avoids the use of carbon fuels. Using very-high-temperature advanced nuclear reactors, such as Generation IV gas-cooled or liquid metal-cooled reactors, nuclear energy can produce hydrogen in very large quantities consistently over long periods of time without emitting greenhouse gases or other harmful air emissions.

200. DEVELOPMENT OF ADVANCED HIGH-TEMPERATURE HEAT EXCHANGERS
$2,000,000
DOE Contact: Carl Sink, 301-903-5131
UNLV Contact: Tony Hechanova, 702-895-1457

The goal of this project is to develop high-temperature heat exchangers for hydrogen production from advanced nuclear reactors. The challenge lies in developing heat exchangers that can withstand very high temperatures (850°C and above) and highly reactive and corrosive process fluids. The working fluids include sulfuric acid, hydrogen iodide, and steam/water as the cold fluids, and helium or molten salt as the hot fluid. Candidate materials for the heat exchangers include the following classes: high-temperature nickel-based alloys, high-temperature ferritic steels (particularly oxide dispersion strengthened), and carbon and silicon carbide composites. Research includes general and localized corrosion studies, tensile testing at high temperatures, TEM, SEM and metallographic examination, stress corrosion cracking tests at elevated temperatures and heat transfer phenomena.

Keywords: Heat Transfer, Heat Exchangers, Ferritic Steels, Composites, Corrosion, Molten Salt, Hydrogen Production

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2004
NATIONAL NUCLEAR SECURITY ADMINISTRATION - GRAND TOTAL	$119,168,000
OFFICE OF NAVAL REACTORS	$75,800,000[1]
OFFICE OF DEFENSE PROGRAMS	$43,368,000
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM	$43,368,000
SANDIA NATIONAL LABORATORIES	$31,935,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$9,496,000
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	350,000
Solution-Based Nanoengineering of Materials	340,000
Assembly and Actuation of Nanomaterials Using Active Biomolecules	500,000
Decomposition of Contaminants Using Photochemically Active Nanoparticles	430,000
Thermally Cleavable Surfactants	300,000
Transition-Metal Catalyzation of Complex-Hydride Absorption/desorption Reactions	201,000
Assembly of Ordered Electro-Optical and Bioactive Materials and Composites	400,000
Active Photonic Nanostructures	500,000
Development of High Energy Density Dielectric Materials for Integrated Microsystems	300,000
Nanolithography Directed Materials Growth and Self-Assembly	400,000
Novel Gel-Based Technology for Sensors and Weapons	100,000
Developing the Foundation for Polyoxo-Niobate Chemistry: Highly Tunable and Exploitable Materials	200,000
Physics and Chemistry of Ceramics	874,000
Field-Structured Anistropic Composites and Complex and Cooperative Phenomena in Disordered Ferroelectrics and Dielectrics	481,000
Artificially Structured Biocompatible Semiconductors	501,000
Atomic Processes and Defects in Wide-Bandgap Semiconductors	378,000
Advanced Growth Techniques and the Science of Epitaxy	307,000
Active Assembly of Dynamic and Adaptable Materials	900,000
The Science of Heteroepitaxial Structural Evolution	480,000
Synthesis and Processing of Nanoclusters for Energy Applications	255,000
Dipolar Nanocomposites	185,000
Cooperative Phenomena in Molecular Nanostructures	539,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$17,154,000
Nanostructured Materials for Directed Transport of Excitation Energy	200,000
Quantification of Environments and Surfaces Within Micro-Packages	400,000
Experimental and Computational Study of Liquid-Solid Transition in Tin	100,000
Electrochemically Switchable Materials for Bio-Microfluidics	200,000
Correlated and Comprehensive Analytical Techniques for Homeland Defense	500,000
Development of a Novel Technique to Assess the Vulnerability of Micro-Mechanical System Components to Environmentally Assisted Cracking	183,000
3D Optical Sectioning with a New Hyperspectral Deconvolution Fluorescence Imaging System	525,000

[1]This excludes $61.1 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2004
OFFICE OF DEFENSE PROGRAMS (continued)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (continued)	
SANDIA NATIONAL LABORATORIES (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
Coupled Nanomechanical Oscillator Arrays for the Study of Internal Dissipation in Nano-Scale Structures and Collective Behavior in Large Systems	330,000
Atomic Level Science of Adhesion and Interfacial Wetting	618,000
Mechanical Properties of Nanostructured Materials	356,000
Localized Corrosion Initiation at Nanoengineered Defects in Passive Films	602,000
The Physics of Structured Semiconductors	485,000
The Science of Electronic and Optical Interactions Between Coupled Nanostructures	505,000
Materials Aging and Analytical Technique Development	4,500,000
Scientifically Tailored Materials and Materials Processing	4,500,000
Nanosciences, Enhanced Surety and Enhanced Use Denial	3,150,000
MATERIALS STRUCTURE AND COMPOSITION	$4,360,000
The Basics of Aqueous Nanofluidics: "Interphase" Structure and Surface Forces	300,000
Modeling Local Chemistry in the Presence of Collective Phenomena	170,000
Modeling of Friction-induced Deformation and Microstructure	485,000
The Science of Solutes: Transition Metals in Liga Nickel	315,000
Dynamics and Structure of Interfaces and Dislocations	2,171,000
Theory of Microstructures & Deformation	168,000
Long Range Particle Interactions and Collective Phenomena in Plasma Crystals	361,000
Atomistic Basis for Surface Nanostructure Formation	390,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$925,000
Advanced Packaging/Joining Technology for Micro	350,000
Magnetostrictive Elastomers for Actuators and Sensors	150,000
Reversible Antibody Trapping for Selective Sensor Devices	200,000
Precisely Controlled Picoliter Vessels with Rapid Sample Preparation for Trace Biotoxin Detection	225,000
LAWRENCE LIVERMORE NATIONAL LABORATORY	$11,433,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$8,500,000
Engineered Nanostructure Laminates	8,500,000
INSTRUMENTATION AND FACILITIES	$2,933,000
AFM Investigations of Biomineralization	113,000
Polyimide Coating Technology for ICF Targets	1,000,000
Beryllium Ablator Coatings for NIF Targets	1,000,000
Using Dip-Pen Nanolithography to Order Proteins and Colloids at Surfaces	420,000
Plasma Polymer Coating Technology for ICF Targets	400,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION

OFFICE OF NAVAL REACTORS

The Deputy Administrator for Naval Reactors within the National Nuclear Security Administration is responsible for conducting requirements under Section 309(a) of the Department of Energy Organization Act which assigns civilian power reactor programs and all DOE naval nuclear propulsion functions. Executive Order 12344, as set forth in Public Law 106-65, stipulates responsibilities and authority of the Naval Nuclear Propulsion Program, of which the Deputy Administrator for Naval Reactors is a part.

The materials program supports the development and operation of improved and longer life reactors and pressurized water reactor plants for naval nuclear propulsion.

The objective of the materials program is to develop and apply, in operating service, materials capable of use under the high power density and long life conditions required of naval ship propulsion systems. This work includes irradiation testing of reactor fuel, poison and cladding materials in the Advanced Test Reactor at the Idaho National Engineering Laboratory. This testing and associated examination and design analysis demonstrates the performance characteristics of existing materials as well as defining the operating limits for new materials.

Corrosion, mechanical property and wear testing is also conducted on reactor plant structural materials under both primary reactor and secondary steam plant conditions to confirm the acceptability of these materials for the ship life. This testing is conducted primarily at two Government laboratories—Bettis Atomic Power Laboratory in Pittsburgh and Knolls Atomic Power Laboratory in Schenectady, New York.

One result of the work on reactor plant structural material is the issuance of specifications defining the processing and final product requirements for materials used in naval propulsion plants. These specifications also cover the areas of welding and nondestructive testing.

Funding for this materials program is incorporated in naval projects jointly funded by the Department of Defense and the Department of Energy. This funding amounts to approximately $136.9 million in FY2004. Approximately $61.1 million represents the cost for irradiation testing in the Advanced Test Reactor.
The Naval Reactors contact is David I. Curtis,
(202) 781-6141.

OFFICE OF DEFENSE PROGRAMS

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

200. DESIGN, SYNTHESIS, AND CHARACTERIZATION OF SOFT MATTER NANOLAYER SUPERLATTICES
$300,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Alfredo M. Morales, 925-294-3540

The second year we focused our efforts on the synthesis of a variety of photoresponsive azobenzene polymers/molecules that were similar to and compatible with polymethylmethacrylate (PMMA), including a non-polymerizable molecule for incorporation into a nanolayer superlattice. A variety of analytical techniques were applied to PMMA blends of the polymers/molecules to select the most promising candidate for subsequent fabrication. These techniques include: UV-Vis absorbtion spectroscopy, ellipsometry, Thermal Mechanical Analysis, microscopy, and spectroscopic examination of heat treated samples. These analytical techniques will lower the technical risk for multilayer fabrication by ensuring that the chromophore chosen for fabrication will have the desired optical properties, will be available in large enough quantities, and will be thermally stable during fabrication. The superlattices will be fabricated by polymeric coextrusion. The coextruder is currently being assembled. The extrusion dies and take up device need to be fabricated. The polarizabilities of the different molecules under consideration are being model at high levels of theory and at different stacking configurations.

Keywords: Superlattices, Birefringent, Nanolayers, Photochromic, Microdevices

201. PHOTO-CONTROL OF NANO-INTERACTIONS IN MICROSYSTEMS
$275,000
DOE Contact: Mike Long, 202-586-4595
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 relying on such nano-interaction-based phenomena as self-assembly, fluid flow, and interfacial tribology. Conventional nano-interaction control strategies typically involve the tailoring of material structures either during synthesis or through invasive post-synthesis processing with no opportunity for real-time, remote modulation of intermolecular and/or interparticle forces. By contrast, the proposed research focuses on the reversible photo-tuning of such interactions through the introduction of photosensitive molecular structures into the material system. This new material strategy provides optical actuation of nano-interactions impacting behavior on both the nano- and macroscales with the potential for impact in directed nanostructure formation, microfluidic rheology, and tribological control.

The work has identified organic structures possessing known photophysical effects with 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 to enable the photo-actuated control of interparticle nano-interactions to reduce the defect content of colloidal crystal arrays (artificial opals). Primary demonstration of successful nano-interaction control will be provided by zone refining of assembled colloidal crystals. A successful demonstration will provide proof that colloidal crystal arrays can be used to form complete photonic band gaps by the elimination of defects which currently prevent band gap development. Extension of these fundamental findings can also provide optically tuned microfluidic rheology and tribological control useful in a range of microsystems with an impact in DOE/DP technologies for stockpile safety and security.

Keywords: Photosensitive, Photonic, Rheology, Polymeric

202. ELECTROCHEMICALLY DEPOSITED ALLOYS WITH TAILORED NANOSTRUCTURES FOR LIGA MICROMACHINES
$350,000
DOE Contact: Mike Long, 202-586-4595
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

203. SOLUTION-BASED NANOENGINEERING OF MATERIALS
$340,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: James Voigt, 505-845-9044

Solution-based synthesis is a powerful approach for creating nano-structured materials. Although there have been significant recent successes in its application to fabricating nanomaterials, the general principles that control solution synthesis are not well understood. We propose to develop the scientific principles required to design and build unique nanostructures in crystalline oxides, II/VI semiconductors, and other technologically significant materials 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 transfrom-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 effect such agents have on interfacial properties. Finally, surface energy calculations based on interatomic potentials will be used to model ligand adsorption on hydrated crystal surfaces. The calculations will be used to design crystallographically specific adsorbate ligands that will be synthesized and tested as surface-specific nucleation promoters and growth inhibitors.

Keywords: Template, Nanostructures, ZnO, Supersaturation

204. ASSEMBLY AND ACTUATION OF NANOMATERIALS USING ACTIVE BIOMOLECULES
$500,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: George Bachand, 505-844-5164

The formation and functions of living materials and organisms are fundamentally different from those of synthetic materials and devices. Synthetic materials tend to have static structures, and are not capable of adapting to the functional needs of changing environments. In contrast, living systems utilize energy to create, heal, reconfigure, and dismantle materials in a dynamic, non-equilibrium fashion. The overall goal of the proposed research is to organize and reconfigure functional assemblies of nanoparticles using strategies that mimic those found in living systems. Active Assembly of Nanostructures will be studied using active biomolecules to create nanowires for programmable interconnects via the on-chip manipulation of gold nanoparticles. In this system, kinesin motor proteins and microtubules will be used to direct the transport of gold nanoparticles on lithographically defined array patterns such that the particles form nanowires and associated interconnects. Responsive Reconfiguration of Nanostructures will be investigated by using active biomolecules to mediate the optical properties of quantum dot (QD) arrays through modulation of inter-particle spacing. Here, the spacing between different sized QDs will be controlled by activation of kinesin motor proteins, and subsequent fluorescence resonant energy transfer will occur between QDs as the inter-particle spacing is changed. In this work we will be able to create and reconfigure synthetic nanostructures using biomimetic process that direct energy consumption to single molecules, and remove diffusional and entropic limitations. The ability to utilize active biomolecules and nanomaterials in integrated systems could revolutionize the exploitation of nanostructured material in complex systems.

Keywords: Biomolecules, Nanowires, Nanoparticles, Functional Assemblies

205. DECOMPOSITION OF CONTAMINANTS USING PHOTOCHEMICALLY ACTIVE NANOPARTICLES
$430,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Kevin McCarty, 925-294-2067

The decomposition of hazardous biological (viruses and bacteria) and non-biological (e.g., nerve agents, H2S, HCN) compounds can be realized using a new class of photochemically active nanoparticles that have been fine-tuned for decontamination applications. Several metal oxides (TiO_2, ZnO, Fe_2O_3, WO_3) have demonstrated the ability to destroy contaminants upon exposure to UV light; however, to make them of practical use improvements in their activity is necessary. These materials work by photo-activating water and oxygen to create highly reactive species (e.g., OH') that readily decompose the compounds described above. Our approach will be to develop highly photo-active, doped, nanomaterials using novel synthetic routes. We will link materials-synthesis studies to understanding the underlying physical mechanisms of these reactions through the use of in-situ microscopy and spectroscopy. These efforts will be coupled to first-principles calculations examining the advantages of likely dopants, followed by a study of reaction processes and statistical mechanical modeling of the reaction dynamics after a material/dopant has been selected. In this manner, the complex inter-relationship between nanostructure, composition, and photochemical activity will be unraveled. Directed by this understanding, sol-gel and surfactant-based supramolecular self-assembly techniques will be used to engineer optimized nanostructures with specified compositions. The photochemical activity of these improved materials will be verified by testing.

Keywords: Nanoparticles, Photo-Active, Materials Synthesis, Decontamination

206. THERMALLY CLEAVABLE SURFACTANTS
$300,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Blake Simmons, 925-294-2067

Surfactants are molecules that have the ability to self-assemble into a variety of supramolecular structures. These structures, and the intrinsic amphiphilic nature of the oil-water interface they possess, have been used in numerous laboratory and industrial processes, including the synthesis of advanced materials. A major problem associated with the use of surfactants is their subsequent removal after use and the recovery of segregated materials. We have successfully developed two novel approaches to surfactant removal using thermally degradable surfactants and metathesis depolymerization that contain weak-links that are internal to the molecule itself. The thermal degradation is based upon a reversible Diels-Alder reaction, which has already found utility at SNL in the preparation of removable encapsulants, foams, adhesives, and dendrimers. The metathesis depolymerization degradation is based upon a catalyzed alkane ring-forming reaction of the surfactant that has been widely used in polymer science.

Surfactant removal becomes very significant in the realm of extended mesoporous nanosized structures, such as ceramics, polymers, inorganic nanocrystals, and polymer-ceramic composites. The present technique of material recovery is typically a combination of centrifugation, calcination, and solvent washing that destroys the desired architecture and functionality of the synthesized material. The incorporation of a cleavable linkage would solve this problem by allowing for the removal of the surfactant molecules through the formation of a hydrophilic and hydrophobic section. These two sections then dissolve into the appropriate phase and are permanently removed from the system through their respective cleaving process. Phase behavior and supramolecular self-assembly of the synthesized surfactants will be computationally modeled and correlated with experimental results to develop a fundamental knowledge of these molecules. Once a working knowledge of these systems is obtained, previously unobtainable extended ceramic, polymeric and composite materials will be synthesized within these systems, recovered after cleavage, and fully characterized.

Keywords: Surfactuants, Mesoporous, Materials Synthesis, Diels-Alder

207. TRANSITION-METAL CATALYZATION OF COMPLEX-HYDRIDE ABSORPTION/DESORPTION REACTIONS
$201,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Eric Majzoub, 925-294-2498

The transformation mechanisms of sodium aluminum hydride ($NaAlH_4$) to its decomposition products of hexahydride Na_3AlH_6, and sodium hydride, NaH are of technological importance. This material is currently of interest to both auto manufacturers and the hydride storage community as a whole for its promising hydrogen weight percentage (around 5 wt.%, more than double the current technology) and its differing nature from the traditional interstitial hydrides.

The material was discovered to be 'reversible' through hydriding and de-hydriding reactions by the addition of a 'dopant', typically a transition metal such as Ti. However, the mechanism, or action, of the dopant is still an open question. This mechanism increases the reaction kinetics by many orders of magnitude, catapulting the material from a standard chemical reducing agent to the forefront of hydrogen storage technology.
Sodium aluminum hydride and other hydrides in this class of materials differ from the classic interstitial hydrides in that these materials have ionic character, with covalently bonded constituents in the atomic cell structure. This is in stark contrast to the 'lattice gas' models used to describe the interstitial hydrides, and new models are here needed. The hydrogen bonding and movement in the bulk structure of these materials is certainly different. It is also dramatically affected by the addition of transition metal 'dopants'.

We propose to continue our development of models and preparation of samples to expose the mechanism and possible defect structures introduced into the lattice by the addition of 'dopant' materials.

The proper understanding of these principles in sodium aluminum hydride may be applicable to a wider range of this class of materials. Because this class of materials also includes compounds with much higher weight percent of hydrogen, there is promise that the Department of Energy goals for over 6-7 wt.% hydrogen can be achieved.

Keywords: Catalysis, Thermodynamics, Metal-hydrides, Hydrogen Storage

208. ASSEMBLY OF ORDERED ELECTRO-OPTICAL AND BIOACTIVE MATERIALS AND COMPOSITES
$400,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Jeffrey C. Brinker, 505-272-7627

The discovery of intrinsic metal-like conductivity in conjugated polymers represents a significant milestone in polymer chemistry and materials science as recently recognized by the 2000 Nobel Prize Award in Chemistry. This project aims to address several key issues related to the performance and utility of conductive polymers. Our objectives are: (1) To develop new methods to assemble ordered conducting materials on multiple length scales. Both self-assembly and directed nucleation and growth approaches will be explored to produce oriented and aligned polymer nanostructures and microstructures. (2) To establish fundamental structure-property relationships of nanostructured conjugated polymers. We propose to investigate films in which conjugated polymers and polymer-nanocrystal composites are confined to ordered structures with 1-, 2-, or 3-dimensional connectivity and separated by either insulating or semiconducting walls. Such composites are ideal model systems in which to test and understand the role of nanostructuring in determining charge and energy transport properties. (3) To integrate the new materials/structures with microelectronic/microfluidic devices. This strategy holds the promise for inexpensive electronic/optical devices.

Micro-arrays of such materials will also be developed for quantitative and high sensitivity detection of chemical and biological agents.

Keywords: Bioactive Materials, Electro-Optics, Microelectronics, Microfluides, Functional Materials

209. ACTIVE PHOTONIC NANOSTRUCTURES
$500,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Michael B. Sinclair, 505-844-5506

Photonic crystals are periodically modulated dielectric structures that alter the flow of electromagnetic energy in many profound and potentially useful ways. Photonic band gaps, transmission resonances, restricted or enhanced densities of states, and modified spontaneous emission rates, are all features of photonic lattices. In general, the photonic crystals demonstrated to date are entirely passive components: there are no means to alter, turn on, turn off, or modulate the unique photonic properties of these structures. The goal of the research project described in this proposal is to integrate these passive photonic crystal structures with active materials to provide "active" functions such as optical amplification, lasing, light switching and steering, optical logic, chemical sensing, etc. In addition to greatly expanding the functionality of photonic crystals, incorporation of active materials will offer new opportunities for investigation of the novel physics arising from the strong modification of the photonic density of states and photonic band structures as they impact electron-photon interactions. A number of approaches to the "activation" of photonic crystals are being explored including fabricating the photonic crystals from active materials such as light emitting materials, nonlinear optical materials, piezoelectric, or electro-mechanical materials. Fabrication efforts include both top-down lithographic approaches as well as bottom-up self-assembly methods. Another approach involves doping of photonic crystal structures such as high-Q resonators with optically active materials such as quantum dots or rare-earth ions. Another approach involves integrating the photonic crystals with active layers of light emitting, piezoelectric or electro-mechanical materials. In addition, energy transfer processes are being investigated for use as a means to couple energy into and out of photonic crystals. This project is a collaboration between Sandia and Los Alamos and draws upon the demonstrated strengths of these institutions in photonic crystal structures, colloidal quantum dots, energy transfer in composite nanomaterials, nanomechanics, and self-assembly.

Keywords: Photonics, Optoelectronics, Photonic Crystals, Active Control, Electro-Optics

210. DEVELOPMENT OF HIGH ENERGY DENSITY DIELECTRIC MATERIALS FOR INTEGRATED MICROSYSTEMS
$300,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Bruce A. Tuttle, 505-845-8026

Next generation surety systems require compact, highly integrated microsystems to improve device functionality, miniaturization, and high-g reliability. Capacitors are by far the largest components in these systems; the greatest increase in volumetric device efficiency can be gained by reducing capacitor size. In the last three years, dramatic developments in dielectric science have been reported that can enable 2X to 100X size reduction in capacitor size over state of the art, commercial materials. We propose in this work to develop these new materials for high field applications, and integrate them into microsystems using direct-write technologies. Two new dielectric materials families will be investigated as alternatives to state of the art K ~ 1100 dielectrics:

1. Specially formulated lead lanthanum zirconate titanate (PLZT), K ~ 2500
While recently developed high Zr content PLZT capacitor materials exhibit twice the pulsed discharge energy of state of the art BaTi03 materials, further improvements of 2X to 4X are anticipated via chemical preparation techniques and combinatorial composition optimization.

2. Novel relaxor dielectrics, with temperature-stable K > 12,000.
A small subset of relaxor dielectric materials, first reported in 2000, have temperature stable relaxor dielectric characteristics that have not been observed previously in any other known materials. For these materials, $CaCu_3Ti_4O_{12}$, Ca:K(Ta,Nb) O_3, and (Pb,La)TiO_3, dielectric constants of 12,000 to 280,000 that are stable over more than a 300ºC temperature range have recently been measured, but have not been integrated or evaluated at high electric fields. These materials could lead to 10 to 100+ times reduction in the size of pulse discharge capacitors.

Sandia is uniquely positioned to develop these microsystem-enabling technologies due to the combined internationally recognized excellence of three different skill sets: (1) fundamental physics of ferroelectrics, (2) direct write technologies for chemically prepared ceramics, and (3) design and fabrication of surety microsystems.

Keywords: Capacitors, Dielectric, Relaxor, DirectWrite

211. NANOLITHOGRAPHY DIRECTED MATERIALS GROWTH AND SELF-ASSEMBLY
$400,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Julia W. P. Hsu, 505-284-1173

The goal of this proposal is to integrate nanotechnology and inorganic materials growth/assembly for potential applications in bio/chemical sensing, optoelectronics, catalysis and novel microsystems. In the past few years, great advances have been made to synthesize complex structures composed of inorganic crystals, particularly via "biomimetic" routes. To include these materials in microdevices and microsystems, they will need to be positioned on the substrates in a controlled and pre-determined fashion. In addition, we need to control the crystal size, morphology, orientation, as well as hierarchical ordering. Conventional photolithography and electron-beam lithography, which are "top-down" fabrication techniques, do not take advantage of crystal growth and self-assembly processes, and they are not adequate for use on these three-dimensional (3D) structures. In contrast, soft nanolithography techniques, e.g., micro-contact printing (CP), nanotransfer printing (nTP) and dip pen nanolithography (DPN), are "bottom-up" approaches. We propose to use these techniques to modify the local surface properties with functional organic monolayers to direct crystal growth/assembly. In interference and two-photon lithography, light will be used to modify local growth conditions in order to make complex 3D structures with patterns spanning nanometer to micrometer scales. All these techniques are capable of achieving nanometer resolution. We will apply them to technologically relevant inorganic crystals, e.g., ZnO, TiO_2, ZnS, as well as self-assembled materials, such as mesoporous silica. With the approaches outlined in this proposal, we will not only produce materials suitable for microsystem integration, but also provide new insight into crystal growth and self-assembly processes at the nanometer scale.

Keywords: Nanolithography, Nanotechnology, Bio/Chemical Sensing, Optoelectronics, Catalysis, Microsystems

212. NOVEL GEL-BASED TECHNOLOGY FOR SENSORS AND WEAPONS
$100,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Joseph L. Lenhart, 505-284-9209

A gel is a cross-linked polymer highly swollen by solvent. Polymer gels undergo a volume phase transition when external conditions such as temperature, pH, solvent, or concentration of chemical or biological analytes, is altered. The focus is to develop a fundamental understanding the volume phase transition in non-aqueous based polymer gels. The research will have two applications. First, this work will provide the scientific foundation necessary to launch Sandia into sensor development for chemical and biological agents, a likely new arena relevant to homeland defense initiatives. Second, this research is essential for developing materials solutions to mitigate aging risks associated with the new gel based capacitors proposed for weapons firing sets.

In sensor applications we will exploit the swelling-shrinking transition in the gel. For example, the gel polymer can be modified with receptor sites specific to particular chemical or biological analytes. Upon receptor-analyte binding, the interactions in the gel change, inducing shrinkage, which is detected by the sensor. The first challenge is to develop a gel that is sensitive to small levels of chemical changes (analyte absorption). The second challenge is to tune the shrinking kinetics to get a rapid sensor response time. The key aspect addressed by this LDRD is to understand the thermodynamics of the phase transition and the impact of the polymer structure on the transition so that the above challenges can be met.

For weapons applications, this work will immediately impact a mission critical stockpile stewardship problem facing the W76-1 and W80-3. The highest risk associated with both refurbishments is the incorporation of new gel-based capacitor technology in the weapon firing sets. A critical aging mechanism for these capacitors is solvent partitioning and surface segregation in the margin-fill gel. A scientific understanding of this partitioning is critical for accurate prediction of capacitor lifetime.

Keywords: Polymer, Polymer Gels, Capacitors, Analyte Absorption, Phase Transition

213. DEVELOPING THE FOUNDATION FOR POLYOXO-NIOBATE CHEMISTRY: HIGHLY TUNABLE AND EXPLOITABLE MATERIALS
$200,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: May D. Nyman, 505-284-4484

The first ~70 years of polyoxometalate (POM) research was dominated by polyoxotungstates, polyoxomolybdates, and more recently polyoxovanadates. Many POM geometries and compositions have been reported; they have been employed in a diversity of applications including virus/protein binding, catalysis, electro-optic and electro-chromic materials, and as building blocks for nano-structured materials. In August 2002, we reported a general synthetic procedure for polyoxoniobates, thus beginning a new branch of POM chemistry, impacting both fundamental understanding and applications of POMs. Even more intriguing, these polyoxoniobates differ significantly from other POMs as a result of much higher surface charges, and base-stability rather than acid-stability.

We will develop the foundation for polyoxoniobate chemistry so that it may become an expanded class of functional materials similar to the other POMs. We will execute this by first understanding the mechanisms of polyoxoniobate formation using in-situ NMR (nuclear magnetic resonance) techniques. Synthesis of new polyoxoniobates will be guided by the NMR studies, as will synthesis of solid-solutions between the polyoxoniobate family and the other POM families. Development of these solid-solutions will give POMs with highly tunable properties including charge and pH stability. In these studies, we will also seek to understand the fundamental differences between the POM families. Additionally, this project will be used to develop ab initio structure determination from X-ray powder data as an integral part of the capabilities of CINT and Sandia.

In summary, execution of the proposed work will allow Sandia to lead the way in establishing polyoxoniobate chemistry, explore avenues for new and improved POM applications, and become one of the few U.S. institutes with ab initio structure determination from powder diffraction as a core capability.

Keywords: Polyoxometalate, Polyoxoniobates, NMR

214. PHYSICS AND CHEMISTRY OF CERAMICS
$874,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: Jun Liu, 505-845-9135 and C. Jeffery Brinker, 505-272-7627

The goal of the program is to develop fundamental understanding of chemical and physical processes that determine structural evolution and structure-property relationships in ceramic materials. Specific scientific issues being addressed include: design and synthesis of complex molecular precursors with controlled architectures, developing novel self-assembled nanomaterials and functions, fundamental understanding of self-assembly mechanisms and structural evolution from molecular level to nano- and microscale, and fundamental understanding of structure-property relationship.

Keywords: Ceramics, Molecular Precursors, Self-Assembly

215. FIELD-STRUCTURED ANISTROPIC COMPOSITES AND COMPLEX AND COOPERATIVE PHENOMENA IN DISORDERED FERROELECTRICS AND DIELECTRICS
$481,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: George Samara, 505-844-6653 and J. E. Martin, 505-844-9125

Task 1- Field-Structured Anisotropic Composites

To create and understand novel ceramic/polymer and metal/polymer composites formed by polymerizing a continuous network-forming phase around particles having an electric permittivity or magnetic permeability mismatch, while subjecting these to uniaxial, biaxial, or triaxial electric or magnetic fields. The applied fields polarize the particles, inducing strong anisotropic forces that have components parallel *and* perpendicular to their line of centers. The resultant field-structured composites can have highly anisotropic mechanical and transport properties, and can be made of a wide variety of materials.

Task 2 - Complex and Cooperative Phenomena in Disordered Ferroelectrics and Dielectrics

The objective of this task is to understand the properties of ferroelectrics and relaxors and of the mechanisms for ferroelectric-to-relaxor crossover in compositionally-disordered ferroelectrics. Some emphasis is on dipolar impurities in quantum paraelectrics and the onset of dipolar correlations. One aspect of this work is the behavior of such systems in the quantum regime and at the displacive quantum limit. This is the limit where $T_c \sim 0$ K and quantum fluctuations come into play, qualitatively changing the nature of the response. Our unique approach emphasizes the use of high pressure to delicately tune the balance between short- and long-range interactions in these systems providing revealing insights into the physics.

Keywords: Cooperative Phenomena, Ferroelectrics, Field-Structured Composites, Ferroelectric-to-Relaxor

216. ARTIFICIALLY STRUCTURED BIOCOMPATIBLE SEMICONDUCTORS
$501,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: Paul Dressendorfer, 505-844-5373 and P. L. Gourley, 505-844-5806

This program investigates biocompatible semiconductor micro/nanocavities for optical sensing of biomolecules and cells. The scope of the program includes semiconductor material design, surface functionalization for biocompatibility, and materials processing and integration into micro/nanocavities. These structures are interfaced with microfluids comprising biomolecules, pathogens, organelles, and whole cells. The goal is to successfully integrate semiconductors, glass, and polymeric materials into functional structures for study and discovery of novel optical transduction methods for sensing biomolecules and micro-organisms. The program emphasizes both scientific and technological impact.

Keywords: Biocompatible Semiconductor, Micro/nanocavities, Microfluids, Optical Transduction

217. ATOMIC PROCESSES AND DEFECTS IN WIDE-BANDGAP SEMICONDUCTORS
$378,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: J. Charles Barbour, 505-844-5517 and S. M. Myers, 505-844-6076

Our objective is fundamental understanding of the atomic processes and point defects that limit the performance of wide-bandgap compound semiconductors. Experiments using a variety of electrical, spectroscopic, and ion-beam analyses are interpreted through quantitative modeling based on ab-initio theory to achieve a unified, predictive description of behavior. The principal current focus is GaN and its alloys with Al and In, where we are investigating the interrelated behaviors of H and point defects and their critical influence on p-type doping. Properties under study include the configurations, state energies, diffusion, and bound complexes of H, point defects, and the Mg acceptor. Analogous experiments have begun on ZnO, a promising wide-gap material where the fundamental issues facing p-doping have proved even more challenging.

Keywords: Point Defects, Wide-Bandgap Compound Semiconductors, Ab-Initio Theory, GaN, ZnO

218. ADVANCED GROWTH TECHNIQUES AND THE SCIENCE OF EPITAXY
$307,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: Neal Shinn, 505-844-5457 and J. A. Floro, 505-844-4708

Develop fundamental scientific understanding of the processes governing thin film growth, epitaxy, and structural evolution using advanced growth techniques coupled with in situ diagnostics, Our current focus is on the interaction of elastic strain with film microstructure and surface morphology, with an increasing emphasis on exploiting our understanding to tailor self-assembly processes.

Keywords: Thin Film Growth, Epitaxy, Elastic Strain, Surface Morphology, Self-Assembly

219. ACTIVE ASSEMBLY OF DYNAMIC AND ADAPTABLE MATERIALS
$900,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: Paul Dressendorfer, 505-844-5373 and B. C. Bunker, 505-284-6892

The objective of this research is to identify and learn how to exploit key strategies used by living systems to develop materials whose assembly and disassembly can be programmed or “self-directed” in controlled environments. The focal point of the project involves studying the behavior of energy-consuming proteins that can assemble materials without being limited by constraints imposed by diffusion or equilibrium processes. Key components include microtubules, which are dynamic nano-fibers that can be assembled and disassembled in response to environmental stimuli, and motor proteins, which “walk” along the microtubules to transport materials to desired locations. The concerted interactions between motor proteins, microtubules, membranes, and target building blocks such as nanoparticles will facilitate the assembly of hierarchical materials that can adapt to changing conditions or even be programmed in fluidic systems. Program components include:

- Dynamic Assembly: microtubule assembly and disassembly
- Active Transport: motor protein modifications and use for nanomaterial transport
- Self-Organization: interactions of motor proteins and microtubules with other materials.

Keywords: Microtubules, Motor Proteins, Nanoparticles, Active Transport, Self-Organized

220. THE SCIENCE OF HETEROEPITAXIAL STRUCTURAL EVOLUTION
$480,000
DOE Contact: Richard Kelley, 301-903-6051
SNL Contacts: Robert M. Biefeld, 505-844-1556 and M. E. Coltrin, 505-844-7843

The overall goal of this project is to understand the evolution of structures arising from heteroepitaxial growth. Current emphasis is on the heteroepitaxy of compound semiconductors. Bonding and lattice mismatch with the substrate introduce strain that must be accommodated by a heteroepitaxial film. In some situations interfacial strain leads to misfit dislocations (degrading the thin-film material properties) or even cracking (rendering it useless). On the other hand, interfacial strain can change the dominant growth mode from 2-dimensional planar growth to spontaneous formation of 3-dimensional islands. If one can take advantage of (or learn how to control and manipulate) such island structures, films with unique optoelectronic properties can be produced. Our studies include diagnosing and mitigating detrimental stress-relief mechanisms, investigating defect reduction techniques such as buffer layers, and producing materials with unique optoelectronic properties by taking advantage of spontaneous nanostructure formation due to strain fields, or directed nanostructure formation using specially designed templates.

Keywords: Heteroepitaxial, Interfacial Strain, Misfit Dislocations, Planar Growth, Islands, Stress-Relief

221. SYNTHESIS AND PROCESSING OF NANOCLUSTERS FOR ENERGY APPLICATIONS
$255,000
DOE Contact: Richard Kelley, 301-903-6051
SNL Contacts: George A. Samara, 505-844-6653 and J. P. Wilcoxon, 505-844-3939

This project develops new synthesis and processing methods for producing chemically pure, highly crystalline, metal and semiconductor nanoclusters with controlled sizes. We also apply analytical tools traditionally associated with organic or polymer chemistry to investigate and understand the fundamental size-dependent properties of these clusters with an emphasis on their interfacial properties important to energy applications such as catalysis, photocatalysis and solid state lighting.

Keywords: Semiconductor Nanoclusters, Size-Dependent Properties

222. DIPOLAR NANOCOMPOSITES
$185,000
DOE Contact: Richard Kelley, 301-903-6051
SNL Contacts: George A. Samara, 505-844-6653 and J. E. Martin, 505-844-9125

The goal of this program is to develop and investigate a class of complex materials we call dipolar nanocomposites, that consist of superparamagnetic (or dielectric) nanoclusters organized into structures of variable dimensionality in a solid matrix, using both directed and self-assembly techniques. In these materials, the formation of structure and/or the physical behavior is dominated by collective classical interactions. Our approach is to understand the physical properties of isolated nanoclusters, how single nanocluster properties change in complex particle assemblies, and how these nanoclusters interact to produce the collective properties observed in nanocomposites.

Keywords: Dipolar Nanocomposites, Superparamagnetic, Dielectric, Variable Dimensionality, Nanoclusters

223. COOPERATIVE PHENOMENA IN MOLECULAR NANOSTRUCTURES
$539,000
DOE Contact: Richard Kelley, 301-903-6051
SNL Contact: Alan R. Burns, 505-844-9642

We seek to establish key scientific principles needed to design and fabricate three dimensional nanocomposite architectures that combine the unique functions and capabilities of organic molecular assemblies and biomolecules with robust, stable inorganic scaffolds. Our research is focused on the interplay between architectures of multiple, hierarchical length scales, cooperative molecular responses, and the resultant overall properties of this new class of organic-inorganic composites. We approach this objective by synthesizing model molecular composites via self-assembly techniques, and by applying unique diagnostic and modeling tools to monitor structure and response directly.

Keywords: Molecular Nanostructures, Inorganic Scaffolds, Hierarchical Length Scales, Cooperative Molecular Responses

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

224. NANOSTRUCTURED MATERIALS FOR DIRECTED TRANSPORT OF EXCITATION ENERGY
$200,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Michael B. Sinclair, 505-844-5506

An extremely desirable functionality for nanostructured materials is the ability to efficiently activate or interrogate structures within a nanoscale device using optical energy. However, given the packing densities obtainable with nanofabrication, direct focusing of incident optical energy onto individual nanostructures is impractical. We will determine how energy transfer phenomena 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. The coupling between the chromophores allows the excitation energy to hop from site to site, until it becomes trapped at a low energy site where it is utilized. In this context, energy transfer networks can loosely be thought of as "lenses" that "focus" optical energy onto a desired site. In addition to initiating chemical, structural or electrical processes, one can envision energy transfer networks that are used for efficient interrogation of the state of selected nanostructural units. In this case, absorbed optical energy is delivered to a fluorescent nanostructure whose emission properties depend upon the local state or environment. In this research program both organic and metallic nano-arrays for energy transfer will be fabricated and characterized. Energy transporting arrays of organic chromophores will be fabricated using Langmuir-Blodgett techniques, crystal growth, and lipid bilayers. Metallic nanoparticle arrays for plasmonic energy transport will be fabricated using self-assembly on suitably prepared insulating substrates.

Keywords: Nanomaterial, Chromophore, Delocalization, Nanolithography

225. QUANTIFICATION OF ENVIRONMENTS AND SURFACES WITHIN MICRO-PACKAGES
$400,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Steven Thornberg, 505-844-8710

Chemical and physical materials-aging processes can significantly degrade the long-term performance and reliability of dormant microsystems. This degradation results from materials interactions with the evolving microenvironment by changing both bulk and interfacial properties (e.g., mechanical and fatigue strength, interfacial friction and stiction, electrical resistance). Eventually, device function is clearly threatened and, as such, these aging processes are considered to have the potential for high (negative) consequences.

Currently, there is no reliable information on the critical species (and concentration levels) that will be present within the sealed packages or on component surfaces. The analytical techniques for properly characterizing these environments do not exist. The goal of this proposal is to develop a set of tools that are analytical strategies and methods to measure the spatially resolved chemical inventory within a Sandia fabricated and packaged microsystem. These tools can be broadly subdivided into surface and internal gas atmosphere characterization, with the aid of multivariate data processing. Both will require design and fabrication of a suitable microelectromechanical system (MEMS) test platform capable of being opened easily and cleanly. Surface characterization will involve labeling (e.g., isotopic, chemical tagging) known contaminants to monitor their movement using enhanced surface analyses. For internal gas characterization, we will develop new micro-volume sampling techniques that provide greatly enhanced sampling efficiency of analytes and couple these to mass spectrometric and optical analysis methods. We will develop and apply new multivariate statistical techniques to spatially resolved ion, x-ray and optical spectroscopies and scanning probe microscopies to identify and quantify the spatial distribution of critical surface species (e.g., lubricants, anti-stiction reagents) and contaminants.

Keywords: Materials Aging, MEMS, Microelectromechanical, Packaging, Surface Analysis, Chemical Analysis

226. EXPERIMENTAL AND COMPUTATIONAL STUDY OF LIQUID-SOLID TRANSITION IN TIN
$100,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Jean Paul Davis, 505-284-3892

The behavior of materials under dynamic high-pressure conditions is directly relevant to stockpile stewardship and is of scientific interest. In particular, there is a programmatic need for improved understanding of liquid-solid phase transition behavior. We propose to study the freezing transition in tin under compression. This continuation proposal focuses future work away from the liquid-liquid transition discussed in the original FY03 proposal, because further analysis of early experiments and new computational results suggest the liquid-liquid transition is not important in tin. The freezing transition, however, has continued to be observed in tin under dynamic compression.

We continued to improve a technique to subject molten metals to a ramped compression wave. Preliminary results suggest a nonequilibrium freezing transition, the rate depending heavily on impurities, and the possibility of a noncrystalline metastable phase. Proposed continuing work will investigate the equation-of-state (EOS) for tin and the kinetics of the solidification process. Continuum models will be developed to aid analysis of the experimental results. We have extensive experience modeling solidification in metallic systems using both atomistic and continuum-level techniques. Proposed continuing work will use ab initio molecular dynamics to determine the EOS and structure of liquid tin as a function of pressure and temperature. In addition, we will investigate the kinetics of solidification using empirical-potential molecular dynamics coupled with continuum-level analytical models.

Keywords: Phase Transition, Freezing, Tin, Dynamic Compression, Molecular Dynamics

227. ELECTROCHEMICALLY SWITCHABLE MATERIALS FOR BIO-MICROFLUIDICS
$200,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Kevin R. Zavadil, 505-845-8442

We propose to develop, characterize and demonstrate the function of a class of materials that can be manipulated at a molecular scale to selectively bind and release a range of biospecies of interest. We will use electrochemical switching to drive the binding and unbinding process using an inclusion complex based on b-cyclodextrin and functionalized ferrocene. Binding specificity can be controlled by modifying ferrocene with a variety of receptor sites. The inclusion complex will be incorporated into microfluidic platforms by deposition onto microelectrodes in fluid channels in MEMS-based devices. In the process of conducting this research, we will develop several new techniques for characterizing and processing functional materials at the molecular level and for conducting electrochemical nanolithography. Our proposed research involves constraining the location of specific biospecies and we will demonstrate how this approach can be combined with a constrained biospecies transport concept of a separate LDRD proposal. Together, a larger scale of controlled manipulation of biospecies will be provided. Importantly, this project will utilize Sandia's expertise in novel materials synthesis, molecular scale characterization, microelectromechanical system (MEMs) design and fabrication, and integrated microfluidics systems. The project will produce the scientific knowledge necessary to design functional engineered surfaces and, in turn, define their viability at the device level. If successful, this strategy would represent a viable foundation for nanoscale, high density, combined molecular level computing and sensing technologies.

Keywords: Biospecies, Electrochemical Switching, Microfluidic, MEMS

228. CORRELATED AND COMPREHENSIVE ANALYTICAL TECHNIQUES FOR HOMELAND DEFENSE
$500,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Paul G. Kotula, 505-844-8947

Identification of unknowns (biological/otherwise) to determine origin or potential threat requires multiple analytical tools covering molecular and elemental signals spanning both organic and inorganic materials. Additionally, each class of analysis may involve multiple independent techniques. While each individual analysis can be interpreted, the challenge arises in correlating all the disparate signals in a self-consistent and statistically rigorous framework-inputting data and getting out knowledge. No tools currently exist that are up to this significant and important challenge. Over the past four years, Sandia has successfully developed a set of multivariate statistical analysis data-mining tools called Automated eXpert Spectral Image Analysis (AXSIA) based on principal components analysis and constrained factor analysis. The specific approach to data analysis embodied by AXSIA has successfully been applied, independently, to x-ray microanalysis, x-ray fluorescence, and time-of-flight mass spectrometry. Significant challenges exist, however, to an even more general application of this approach to the simultaneous correlation of the analytical signals required for the comprehensive analysis of unknowns. This work will address firstly data acquisition/aggregation of multiple analytical signals from test and surrogate bio-weapon materials covering a range of possible analyses. Secondly this work will address computational and algorithm-development issues for the analysis of what are anticipated to be 20Gbyte+ super data sets. Algorithm development will focus on developing efficient multivariate statistical analysis algorithms with more complex constraints and novel data-weighting methods that are capable of handing the expected disparate types of information, sensitivities, signal-, noise- and significance-characteristics.

Keywords: Multivariate, Spectral Image Analysis

229. DEVELOPMENT OF A NOVEL TECHNIQUE TO ASSESS THE VULNERABILITY OF MICRO-MECHANICAL SYSTEM COMPONENTS TO ENVIRONMENTALLY ASSISTED CRACKING
$183,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: David G. Enos, 505-844-2071

Microelectromechanical systems (MEMS) will play an important functional role in future DOE weapon and Homeland Security applications. If these emerging technologies are to be applied successfully, it is imperative that the long-term degradation of the materials of construction be understood. Unlike electrical devices, MEMS devices have a mechanical aspect to their function. Some components (e.g., springs) will be subjected to stresses beyond whatever residual stresses exist from fabrication. These stresses, combined with possible abnormal exposure environments (e.g., humidity, contamination-, introduce a vulnerability to environmentally assisted cracking (EAC). EAC is manifested as the nucleation and propagation of a stable crack at mechanical loads/stresses far below what would be expected based solely upon the materials mechanical properties. If not addressed, EAC can lead to sudden, catastrophic failure. Considering the materials of construction and the very small feature size, EAC represents a high-risk environmentally induced degradation mode for MEMS devices. Currently, the lack of applicable characterization techniques is preventing the needed vulnerability assessment. The objective of this work is to address this deficiency by developing techniques to detect and quantify EAC in MEMS materials and structures. We propose to generate fully instrumented specimens using electrochemical and thin-film processing techniques. These structures will be evaluated by integrating state-of-the-art fracture mechanics instrumentation, sub-pA electrochemical measurement capabilities, and precise control of atmospheric conditions. This approach will allow real-time detection of crack initiation and propagation. The information gained will establish the appropriate combinations of environment (defining packaging requirements), local stress levels, and metallurgical factors (composition, grain size and orientation) that must be achieved to prevent EAC.

Keywords: Residual Stresses, Failure, Degradation, Fracture, Crack Initiation

230. 3D OPTICAL SECTIONING WITH A NEW HYPERSPECTRAL DECONVOLUTION FLUORESCENCE IMAGING SYSTEM
$525,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: David M. Haaland, 505-844-5292

We propose to design, build, and apply a novel hyperspectral deconvolution fluorescence microscope for 3-D diffraction-limited optical sectioning of cells and subcellular organelles, 3-D monitoring of microfluidic processes, and investigation of molecular motors. We will develop data analysis methods to deconvolve the hyperspectral image data and to rapidly extract 3-D concentration distribution maps of all emitting species. The imaging system will have many advantages over current confocal imaging systems: simultaneous monitoring of numerous highly overlapped fluorophores, immunity to autofluorescence or impurity fluorescence, enhanced sensitivity, and dramatically improved accuracy and dynamic range. Combining our patented multivariate curve resolution analysis with deconvolution of hyperspectral images will improve the deconvolution process. The system will make rapid survey scans of large areas followed by detailed 3-D composition maps of small targeted volumes at high spatial and temporal resolutions. Efficient data compression in both the spatial and spectral dimensions will allow PCs to perform quantitative analysis of hyperspectral images of size >10 gigabytes without loss of image quality. The new imaging system will be an enabling technology for numerous applications including (1) 3-D composition mapping analysis of multicomponent microfluidic processes such as mixing, dispersion, and chemical syntheses of materials such as quantum dots, (2) quantitative analysis and co-localization of molecular machines in 3 dimensions, (3) examining the binding of functionalized lipid vesicles to specific cells and the release and/or internalization of the vesicle contents, (4) monitoring multiple targets in situ to visualize gene expression, complex pathways, and signal transduction networks in cells, thereby improving our understanding of host response to toxins and pathogens, allowing identification of infection, and speeding the development appropriate treatments for biothreats, and (5) creating better biosensors with multiplexed bead-based assays.

Keywords: Hyperspectral, Fluorescence, Microfluidic, Confocal Imaging, Multivariate

231. COUPLED NANOMECHANICAL OSCILLATOR ARRAYS FOR THE STUDY OF INTERNAL DISSIPATION IN NANO-SCALE STRUCTURES AND COLLECTIVE BEHAVIOR IN LARGE SYSTEMS
$330,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: John P. Sullivan, 505-845-9496

Controlling energy dissipation in nanostructured materials is a fundamental materials issue for Sandia's future micro- and nanosystems. The goal of this project is to understand internal dissipation in structures of nano-scale dimensions. We will use a new approach, the study of large arrays of coupled nanomechanical oscillators combined with theoretical calculations aimed at identifying atomistic mechanisms of dissipation. This research would be directly relevant to the nanomechanics thrust area of the Center for Integrated Nanotechnologies (CINT) and to the development of nanomechanical resonators for homeland security applications (e.g., sensors). Measurements will be made at low temperatures where dissipation due to tunneling states and ballistic phonon transport become important, and a new theoretical approach will be developed that combines large scale classical force field techniques together with first principles quantum mechanical calculations to identify the dissipative defects, such as the ubiquitous tunneling states defects in amorphous materials. In addition, the large system of coupled nanomechanical elements provides a unique experimental platform for understanding major problems in solid state and statistical physics. Coupled oscillator arrays, which resemble two-dimensional (2D) ball-and-spring models, can be used to study disorder-induced localization in 2D systems and stochastic resonance and non-linear effects in coupled systems. Specifically, we will examine localization of vibrational modes of the array at intentionally-introduced defects and coupling of these modes to mechanical noise leading to mode amplification (stochastic resonance) or the emergence of complex phenomena in the case of bistable oscillator arrays (which are a mechanical analog to biological neural networks).

Keywords: Dissipation, Nanostructured Materials, Nanomechanical Oscillators

232. ATOMIC LEVEL SCIENCE OF ADHESION AND INTERFACIAL WETTING
$618,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: Neal Shinn, 505-844-5457 and J. E. Houston, 505-844-8939

To develop an atomistic understanding of the chemical and physical interactions that control solid/solid and solid/liquid interface formation, thereby enabling us to: (1) develop predictive models for adhesive bond strength, interfacial stability, and flow kinetics; and (2) tailor material surfaces for optimized adhesion, wetting or lubrication.

Keywords: Adhesion, Wetting, Interface Formation, Interfacial Stability

233. MECHANICAL PROPERTIES OF NANOSTRUCTURED MATERIALS
$356,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: J. Charles Barbour, 505-844-5517 and D. M. Follstaedt, 505-844-2102

The goal of this project is to achieve fundamental understanding of deformation and stress evolution in nanostructured materials. We determine the fundamental strength mechanisms governing the mechanical properties of metals with ~1-100 nanometer internal structures (grains, second phases), and we identify the fundamental causes of stress during growth of thin films. To accomplish these, we use special syntheses (pulsed-laser deposition (PLD), ion implantation, electrodeposition and lithography), advanced characterizations (nanoindentation + finite) element modeling, MEMS-based testers) and in situ examinations (TEM during straining, specimen curvature during growth).

Keywords: Deformation, Stress Evolution, Laser Deposition, In Situ Examinations

234. LOCALIZED CORROSION INITIATION AT NANOENGINEERED DEFECTS IN PASSIVE FILMS
$602,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contacts: J. Charles Barbour, 505-844-5517 and N. A. Missert, 505-844-2234

Develop quantitative understanding of the mechanisms of localized corrosion initiation in passive metals using nanofabrication techniques to create controlled defects and advanced characterization and modeling tools to understand the role of defects in pit initiation.

Keywords: Localized Corrosion, Nanofabrication, Pit Initiation

235. THE PHYSICS OF STRUCTURED SEMICONDUCTORS
$485,000
DOE Contact: William Oosterhuis, 301-903-4173
SNL Contacts: J. Charles Barbour, 505-844-5517 and M. P. Lilly, 505-844-4395

To understand the physics of structured semiconductors from the quantum to the macroscopic level. The ultimate goal is to understand how structuring on the nanoscale produces new semiconductor-material properties: optical, electronic, transport and structural. When this goal is achieved, the community will be able to tailor and control the properties of individual electrons and photons with an unprecedented degree of precision, at the level of the wavefunction. To this end, this program utilizes three approaches: 1) investigate fabricated quantum confined structures to probe the fundamental physics;
2) investigate the structure of defects in III-Nitrides connecting electronic structure to experimental measurements; and 3) investigate self-assembled nanostructured semiconductors.

Keywords: Wavefunction, III-Nitrides, Electronic Structure, Nanostructured Semiconductors

236. THE SCIENCE OF ELECTRONIC AND OPTICAL INTERACTIONS BETWEEN COUPLED NANOSTRUCTURES
$505,000
DOE Contact: William Oosterhuis, 301-903-4173
SNL Contact: Jerry A. Simmons, 505-844-8402

From a science point of view, some of the most exciting developments at the forefront of condensed matter physics have been the observation of unexpected novel electronic ground states arising from strong interactions, such as the fractional quantum Hall effect. This project seeks to extend the fundamental science, both experimental and theoretical, of interacting nanoelectronic and nanophotonic structures. We will investigate what novel types of behavior ensue from different types of strong nanostructure interactions (tunneling, Coulomb exchange), the sensitivity of this behavior to geometry, temperature, and interaction strength, and methods for producing strongly interacting arrays of nanostructures, including self assembly. The project is organized into three tasks: (1) Interactions of nanoelectronic structures, (2) Interactions of nanophotonic structures, and (3) Hybrid Interactions between nanoelectronic and nanophotonic structures. These tasks are supported by novel nanofabrication approaches.

Keywords: Fractional Quantum Hall Effect, Nanoelectronic, Nanophotonic, Coulomb Exchange, Hybrid Interactions

237. MATERIALS AGING AND ANALYTICAL TECHNIQUE DEVELOPMENT
$4,500,000
DOE Contact: Syed Zaidi, 301-903-3446
SNL Contact: Richard J. Salzbrenner, 505-844-9408

The first main objective of this program is to identify the fundamental chemical and physical mechanisms that cause materials properties to change with time. The knowledge developed provides the foundational understanding required to enable engineering-focused Enhanced Surveillance Campaign tasks to predict the effects of materials aging on nuclear weapon component and system performance. This objective is focused on three areas: 1) Reliability of microsystem materials, which provides the underlying understanding of the microstructural mechanisms and topographical features that control mechanical and tribological behavior of materials; 2) Environmental degradation of metals, which enhances the mechanistic knowledge needed to assess the effects of environmentally induced degradation of metallic components; and 3) Polymer degradation, which improves our capability to predict the reliability and failure of bulk polymeric materials and interfaces that contain polymer-based adhesives and encapsulants.

The second objective is to develop the technology required to reveal the chemical and physical mechanisms that cause materials properties to change with time. Improving our ability to detect the signature of aging in materials through microstructural measurements, correlated information extraction from multiple spectroscopic techniques, and improved sensitivity to low-level chemical signals is essential to a better understanding of materials aging. This objective focuses on: 1) Advances in microstructural and chemical analysis techniques to probe the changes in materials; and 2) Information extraction methods for optimizing the knowledge content from a variety of spectral data sets.

Keywords: Enhanced Surveillance, Reliability, Degradation, Chemical Analysis, Information Extraction

238. SCIENTIFICALLY TAILORED MATERIALS AND MATERIALS PROCESSING
$4,500,000
DOE Contact: Kimberly S. Budil, 202-586-7831
SNL Contact: Grant S. Heffelfinger, 505-845-7801

This goal of this program is to enable performance-based product specification, design, and production in support of the Dynamic Materials Properties campaign, by developing the fundamental understanding of the relationships between materials processing conditions, microstructure, and materials properties for metals, polymers, and ceramics. This activity provides the scientific basis for sound technical decisions about non-nuclear materials and components for the stockpile, and supports potential decisions regarding the choice of replacement materials and the means of manufacturing replacement components. This project focuses on stockpile materials and processes with the highest leverage and greatest uncertainties. These materials include metals, active ceramics, polymers and foams, and special materials. Important materials processes include materials synthesis, forming, fabrication, joining and microsystem fabrication, as well as synthesis and characterization of nanoscale structures.

This program develops a quantitative understanding of how processing variables determine the microstructure and composition of materials that ultimately control critical performance properties. The technical effort determines not only the mean values of these properties, but also their distribution as a result of processing variability so that the margins of performance set by physics and engineering design requirements are quantified. This effort is structured into two areas: 1) Materials development, which addresses the need for characterization of materials with specific properties or performance characteristics to be used in the enduring stockpile; and 2) Materials processing, which supports the robust fabrication of nuclear weapon components.

Keywords: Scientifically Tailored, Active Ceramics, Polymers and Foams, Materials Synthesis, Joining

239. NANOSCIENCES, ENHANCED SURETY AND ENHANCED USE DENIAL
$3,150,000
DOE Contact: Kevin C. Greenaugh, 202-586-2026
SNL Contact: Charles Barbour, 505-844-5517

In support of the Enhanced Surety Campaign, we discover physical principles and assess their utilization in future Nuclear Weapons (NW) technologies. The nanoscience effort is the underlying research and development for enhanced performance in control and safety of NW (enhanced use denial and surety). The work is focused on impacting the predictable performance of safety systems and initiation systems. Specifically, this work evaluates mechanical and optoelectronic devices performance derived from materials properties for these devices and with a particularly strong emphasis on the use of optical properties for enhanced safety. This work includes discovery of physical principles and the application of these discoveries to new devices. A limited amount of this work supports further understanding of radiation effects in optoelectronic materials and supports understanding mechanical properties of LIGA materials. Further, work is done to evaluate energy storage and delivery from potential future systems with a smaller footprint than current systems and with safer architectures. This work includes evaluation of device elements and performance evaluation of advanced firesets, and assessment of radiation-susceptibility of devices. In order to assure the performance and longevity of surety solutions for stockpile refurbishments, the fundamental physical and chemical behaviors of nanostructured materials and optical devices are being investigated for direct or potential use in surety components.

Keywords: Enchanced Surety, Nanoscience, Optoelectronic, LIGA, Radiation-Susceptiblity

MATERIALS STRUCTURE AND COMPOSITION

240. THE BASICS OF AQUEOUS NANOFLUIDICS: "INTERPHASE" STRUCTURE AND SURFACE FORCES
$300,000
DOE Contact: Mike Long, 202-586-4595
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

241. MODELING LOCAL CHEMISTRY IN THE PRESENCE OF COLLECTIVE PHENOMENA
$170,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Normand 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 propose 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 will 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 cannot model CS reliably, while QM methods alone are incapable of treating the extended length and time scales characteristic of CP. Research in this area has been neglected in favor of work on the classical-to-continuum coupling. 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). Previous efforts along these lines have used a simplified, empirical QM model and thus are limited to a narrow range of materials. In contrast, our first-principles approach has the potential to impact numerous mission critical Sandia programs. 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

242. MODELING OF FRICTION-INDUCED DEFORMATION AND MICROSTRUCTURE
$485,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Somuri V. Prasad, 505-844-6966

Frictional contact results in surface and subsurface damage that could influence the performance, aging, and reliability of moving mechanical assemblies. Changes in the surface roughness, hardness, grain size and texture often occur during the initial run-in period, resulting in the evolution of subsurface layers with characteristic microstructural features that are different from the bulk. Recent research on electroformed nickel has revealed the bending of columnar grains, generation of low-angle boundaries, and formation of nanocrystalline zones as a result of sliding contact. We propose to develop models to predict the microstructural changes and debris generation during sliding contact, and validate them with novel experimental techniques. Models will focus on the plastic work in the near surface regions due to the Hertzian contact forces and include work hardening, recovery and the microstructure evolution during sliding contact. Initially, we shall focus on single asperity contact on single crystal surfaces, and extend the work to polycrystalline materials. The influence of friction-induced strains (elastic and plastic) on coating/substrate interface reliability will be incorporated. Model validation will be performed by conducting friction tests on select microsystems materials, and by analyzing the microstructures underneath the wear scars using electron backscatter diffraction and TEM. Cross sections of wear scars, suitable for transmission electron microscopy will be produced in precise locations by focused ion beam micromachining. These results will allow direct comparison with the model predictions and provide a more complete understanding of the friction and wear phenomena in regimes relevant to both micro- and macro-systems.

Keywords: Friction, Electroformed Nickel, Hertzian Contact Forces, Microsystems, Microstructures

243. THE SCIENCE OF SOLUTES: TRANSITION METALS IN LIGA NICKEL
$315,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Albert A. Talin, 925-294-1445

All engineered materials contain solutes, whether intentional (alloying elements) or unintentional (impurities). Although solutes control both the processing and the properties of most alloys, material and process models almost never include their effects. In this project, we make the first concerted effort to include realistic solute effects in mesoscale material models. Novel, LIGA-fabricated nickel-manganese electrodeposits are prime candidate materials for stockpile microsystems applications that require high strength and ductility. Incorporating small amounts of transition metal (TM) dopants in LIGA nickel dramatically suppresses recrystallization and grain growth, preserving the fine-grained as-deposited microstructure throughout subsequent processing. How TMs do this is unknown; nucleation inhibition (via subgrain pinning), enhanced twinning (via decreased stacking fault energy), and growth inhibition (via boundary drag) have been proposed. We shall use state-of-the-art ab initio simulations to characterize the energetics and kinetics of solute segregation and boundary/solute equilibrium for realistic subgrain, twin, and grain boundaries. Using the resulting thermodynamic and kinetic parameters, a 3D digital kinetics model will simulate boundary motion in realistic, multiscale nickel polycrystals containing various TMs. By comparing subgrain, twinning, and grain growth processes, this model will determine recrystallization retardation and texture development mechanisms for a spectrum of nickel-TM alloys. A suite of annealing experiments and mechanical tests will elucidate grain growth, twinning, recrystallization, texture development, and properties for these alloys, to guide and validate the simulations.

Keywords: LIGA, Recrystallization, Grain Growth, Solute Segregation

244. DYNAMICS AND STRUCTURE OF INTERFACES AND DISLOCATIONS
$2,171,000
DOE Contact: Robert Gottschall, 301-903-3978
SNL Contact: Douglas L. Medlin, 925-294-2825

This program seeks to establish the fundamental mechanisms that control the evolution and stability of surfaces and internal interfaces in materials and that dictate how such interfaces interact with their surrounding environment. To accomplish this we tightly couple both experiment and theory. Our experimental effort employs a suite of surface and bulk microscopies, including low energy electron and scanning tunneling microscopy, transmission electron microscopy, and atom probe tomography, that are generally capable of atomic resolution in one or more dimensions, and that often provide new insights through dynamic, *in situ* observations. Our computational effort encompasses a comprehensive set of methods ranging across accurate first-principles electronic structure techniques, semi-empirical atomistic methods, and continuum elasticity and rate equation simulations. In general, we seek to determine how elementary, atomic-scale structures and processes are related to the longer-range interactions that ultimately control interfacial behavior and properties. Thus, for instance, we concentrate significant effort on determining how collective groupings of atoms, such as dislocations and steps, bridge between atomic and macroscopic length scales. In studying the response of interfaces to their surroundings, we seek to explain the interactions of interfaces with both the external environment and the interior bulk of the solid. Such issues are central to materials science and of direct relevance to long-standing and emerging issues in energy science and technology. For instance, gas sensors, gas-separation membranes, and solid-state hydrogen storage rely on surface reactions and interfacial mass transport through the bulk. Catalyst performance depends both on tailoring the surface structure and composition of metal particles and on ensuring the stability of the particle size and morphology on its support. Structural alloys for high temperature applications such as combustion require that the internal microstructure of grain boundaries and heterophase interfaces be stable and that the surfaces be resistant to high temperature degradation processes such as oxidation. By investigating the basic mechanisms that underpin the behavior of surfaces and interfaces, using carefully controlled model systems, we seek to establish basic principles and to discover new phenomena that will have impact across these and other materials issues.

Keywords: Surface and Interface, Dislocations, Grain Boundaries, Microstructure Evolution, Self-Assembly, Microscopy, Theory and Modeling

245. THEORY OF MICROSTRUCTURES & DEFORMATION
$168,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contact: Elizabeth A. Holm, 505-844-9781

The goal of this program is to combine experiment, modeling, and simulation to construct, analyze, and utilize three-dimensional (3D) polycrystalline microstructures. A genetic algorithm, MicroConstructor, is utilized to build 3D polycrystals in a physically correct manner so as to match an arbitrary number of microstructural parameters. The resulting microstructures are input into network analysis models to characterize the microstructural network parameters that influence material properties. Finally, these microstructures provide input for microstructural evolution and response simulations on the grain and subgrain scales. These simulations are targeted toward understanding microstructural effects in polycrystals with the most realistic structure, crystallography, and boundary properties yet studied. This program supports the LANL initiative, “Ensemble-Controlled Deformation Behavior in Materials.”

Keywords: Microstructures, Microstructural Network Parameters, Grain and Subgrain, Deformation

246. LONG RANGE PARTICLE INTERACTIONS AND COLLECTIVE PHENOMENA IN PLASMA CRYSTALS
$361,000
DOE Contact: Yok Chen, 301-903-4174
SNL Contact: Greg A. Hebner, 505-844-6831

Develop fundamental scientific understanding of the long range and collective interactions responsible for the formation of plasma crystals; orderly arrangements of particles that self-assemble in electrical plasmas. Our current focus is on the development of general methods to describe the many-body interactions, diagnostics to characterize the interparticle potentials, and general techniques to model large collective assemblies. We are combining experimental and theoretical studies to develop a mature understanding of the fundamental long-range interactions and multi-particle dynamic behavior within general macroion crystals, of which plasma crystals are one example. We have observed a number of previously unreported and/or uncharacterized plasma crystal behaviors that will have a significant impact on current understanding.

Keywords: Collective Interactions, Plasma Crystals, Many-Body Interactions, Macroion Crystals

247. ATOMISTIC BASIS FOR SURFACE NANOSTRUCTURE FORMATION
$390,000
DOE Contact: William Oosterhuis, 301-903-4173
SNL Contacts: Neal Shinn, 505-844-5457 and G. L. Kellogg, 505-844-2079

Our goal is to establish the scientific principles governing the formation and stability of nanostructures on surfaces. The primary objective is to understand how atomic-scale, kinetic processes control collective surface phenomena such as surface self-assembly, phase transitions, and thermal smoothing. In numerous systems the interplay between the macroscopic thermodynamic properties of surfaces and the microscopic kinetic behavior of adsorbed atoms and clusters produces changes in surface structure and morphology at length scales directly relevant to emerging nanotechnologies. To understand the novel physics resulting from thermodynamics and kinetics acting jointly, we combine low energy electron microscope (LEEM) measurements of the time-evolution of nanoscale surface features with scanning tunneling microscope (STM) and theoretical studies of how atoms and molecules move and interact on surfaces.

Keywords: Collective Surface Phenomena, Surface Self-Assembly, Thermal Smoothing, Surface Structure

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

248. ADVANCED PACKAGING/JOINING TECHNOLOGY FOR MICRO
$350,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Charles V. Robino, 505-844-6557

It is generally agreed that current microelectronics packaging technologies are inadequate for potential microsystems applications. Additionally, the capability to join MEMS components into complex, 3-dimensional assemblies, will be necessary for stockpile applications. Proof-of-concept experiments have identified two complementary new technologies - micron-scale high energy density (HED) fusion welding and focused-ion-beam deposition joining (FIBDJ) - that could jointly address these key microsystem needs. At the micron scale, materials properties which dominate joining response will differ from those at macroscopic sizes. This project is identifying and quantifying the materials properties/process interactions which control microscale joinability in HED welding and FIBDJ.

Microscale HED welding is being studied with concurrent experimental and modeling approaches. Laser and electron beams are being characterized spatially and temporally, and in terms of energy transfer. Previous modeling has shown that melt ejection may preclude joining at <100 micron beam diameters, but did not incorporate the effect of surface tension. Model improvements are incorporating this effect and use Molecular Dynamics simulations to provide surface tensions. Surface Evolver (SE) simulations will guide experiments, and determine if recoil pressure can be used to aid coalescence. Expected results are quantitative mechanistic descriptions of microscale fusion welding, and definitions of microscale weldability.

FIBDJ is being evaluated as an alternative approach. Experiments include characterization of operating parameters, joint geometry, energy transfer, and development of microstructure and properties. Interpretation of microstructural evolution, and its relation to FIBDJ processing are being aided by Kinetic Monte Carlo modeling. The models will be used to derive quantitative mechanistic descriptions of micron and sub-micron size FIBDJ connections and to optimize processing. Residual stress and distortion is expected to be a key issue. We will address its impact at the latter stages of the program, at which time we will draw on existing NW-funded work at the sub-mm size scale.

Keywords: Advanced Packaging, Microscale Welding, MEMS, Focused Ion Beam

249. MAGNETOSTRICTIVE ELASTOMERS FOR ACTUATORS AND SENSORS
$150,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Dale L. Huber, 505-844-9194

There is a need for soft actuators that have a much larger response than piezoelectrics, and that can respond in microseconds. Applications include artificial muscles in robots and stress/strain sensors based on permittivity or permeability changes. We have shown theoretically that large magnetostrictive effects can be obtained from composites of magnetic nanoparticles in an elastomer, if the nanoparticles have been preorganized into chain-like agglomerates using magnetic fields. Such Magnetostrictive Elastomers (MEs) have a magnetic permeability that increases rapidly with compression, and so contract in a magnetic field, providing the particles are spaced by a soft matrix. This effect should be especially large for nanoparticles, where calculations show that the stresses should be comparable to that of human muscle. "Latched" MEs could also be made with particles having large magnetic remanence. A short magnetic pulse would magnetize the particles, causing permanent composite contraction without further power consumption, until an opposing coercive pulse removes the magnetization, releasing the contraction. One challenge in realizing MEs is preventing contact between magnetic nanoparticles during chaining. The most effective method of precoating the nanoparticles with a thin layer of low-modulus elastomer is through a surface-initiated polymerization, wherein an initiating group covalently linked to the surface is used to grow polymers in situ, forming a defect-free coating. MEs should have wide application as large strain actuators, and as soft sensors for robotic fingertips. We expect strains that are 10-100x that of piezoelectrics, and stress response times limited only by the inductance time of the coil.

Keywords: Magnetostrictive Elastomers, Magnetostriction, Permeability, Magnetism

250. REVERSIBLE ANTIBODY TRAPPING FOR SELECTIVE SENSOR DEVICES
$200,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: Dale L. Huber, 505-844-9194

The most sensitive and selective materials for binding and detecting bio-agents are antibodies. Many sensor technologies rely on tethered antibodies for interacting with bio-species. Unfortunately, each antibody is selective to only one antigen. As antibody-antigen complexes form, active sites are consumed, limiting use to one analysis cycle. This LDRD proposal involves studying concepts for producing antibody monolayers that can be regenerated and reused. The baseline concept involves using Sandia's "reversible protein trap" to adsorb and release highly selective antibody monolayers. The protein trap consists of a microhotplate onto which a thermally-activated polymer (PNIPAM) film is tethered. The hotplate is used to switch PNIPAM between a room-temperature phase that repels proteins and a higher-temperature phase that adsorbs proteins (in this case antibodies-. The scientific component of the proposed work will involve using surface-sensitive fourier transform infrared (FTIR), interfacial force microscopy, and neutron scattering measurements to determine: 1) the extent and kinetics of antibody adsorption on activated PNIPAM vs. solution conditions (e.g., competition with other proteins), 2) surface concentrations and orientations of the antibodies, 3) antibody-antigen interactions vs. monolayer structure, and 4) the extent and kinetics of release of antibody-antigen complexes from deactivated PNIPAM films, allowing the surface to be refreshed with the same or a different antibody. The technical component of the work will involve integrating the reversible protein trap into Sandia's highly mass-sensitive shear horizontal surface acoustic wave sensors to make a compact device in which selective capture, sensing, and release functions are all performed in the same location. This investigation of concepts for using switchable, "non-selective" surfaces to adsorb monolayers of highly selective agents will impact a wide range of evolving on-chip separation and sensor systems.

Keywords: Antibodies, Monolayers, Protein Trap, On-Chip Separation, Sensor Systems

251. PRECISELY CONTROLLED PICOLITER VESSELS WITH RAPID SAMPLE PREPARATION FOR TRACE BIOTOXIN DETECTION
$225,000
DOE Contact: Mike Long, 202-586-4595
SNL Contact: C.R. Bowe Ellis, 925-294-2158

We propose to develop novel materials and microfluidic processing technology to chemically process samples within picoliter chambers that are actively moved inside a microfluidic network and controlled solely with induced electric fields. These chambers are phospholipid vesicles, 1-20 microns in diameter, which can be electroformed from synthetic lipids or created from preexisting cells (e.g., ghost RBCs) due to their size and composition, vesicles serve as ideal biomimetic nanoenvironments for rapid, surface-functionalized chemical kinetics. The vesicles will be electrokinetically moved through the fluidic network to specific locations on the chip for loading proteins or analytes via electroporation, a technique in which the bilayer membrane is rendered temporarily porous under an applied electric field. A loading site is designed to allow a single vesicle to come in contact with a loading inlet; electrodes across the vesicle measure its presence as a change in impedance and then electroporate the vesicle. Molecules may be loaded through the porous membrane into the aqueous intravesicular space by mechanism of diffusion or electrophoresis. Each "container" can go through its own series of loading/unloading steps and chemical reactions such that the system functions as a factorial "micro-bucket brigade" for sample preparation and direct assaying. If desired, selected vesicles can be combined to share information via electrofusion. Electroporation parameters can be chosen such that, prior to analysis, excess dye and byproducts are removed from a vesicle via diffusion while not allowing macromolecules to escape. As containers, the vessels will prevent a sample from diluting and reduce mixing volumes. As substrates, vesicles will be ideal for fast surface-dominated reactions required in the preparation of any assay.

Keywords: Picoliter, Microfludic, Phospholipid, Electrokinetically, Membrane

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

252. ENGINEERED NANOSTRUCTURE LAMINATES
$8,500,000
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, energetic materials development, advanced optics development and scientific studies of compound and alloy thermodynamics.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately >50 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: IR, Vis, UV, EUV, soft X-ray and X-ray optics for spectroscopy and imaging; energetic materials, high performance capacitors for energy storage; capacitor structures for industrial applications; high strength materials; integrated circuit interconnects; projection X-ray lithography optics, light weight optic systems.

Keywords: Precision Thin Films; Multilayer/Nano-Laminate Technology; Energetic Materials; IR, Visible, UV, EUV, SXR and XR Optics and Optic Systems, Advanced Joining Techniques, Rapid Manufacture of Lightweight Space Optics, EUV Lithography, Energetic Structural Materials, Armor

INSTRUMENTATION AND FACILITIES

253. 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

254. POLYIMIDE COATING TECHNOLOGY FOR ICF TARGETS
$1,000,000
DOE Contact: Bharat Agrawal, 301-903-2057
LLNL Contacts: R. Cook, 925-422-3117 and Steve Letts, 925-422-0937

This program has as its objective the development of a vapor deposition based polyimide coating technology to produce a smooth 150 μm polyimide ablator coating on a 2mm diameter capsule target for the National Ignition Facility (NIF). The approach involves first vapor depositing monomeric species to form a polyamic acid coating on a spherical hollow mandrel. The surfaces of these coated mandrels are then smoothed by exposure to dimethyl sulfoxide vapor while being levitated on a nitrogen gas flow. The smoothed shells are then heated *in situ* to imidize the coatings. During the past year shells with surfaces that meet the design requirements for NIF targets have been produced. The program was completed at the end of FY04.

Keywords: Polymers, Laser Fusion Targets, Polyimide, Ablator

255. BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS
$1,000,000
DOE Contact: Bharat Agrawal, 301-903-2057
LLNL Contacts: R. Cook, 925-422-3117, R. Wallace, 925-423-7864 and M. McElfresh, 925-422-8686

This program has as its objective the development of materials and processes that will allow sputter-deposition of up to 170 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

256. 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

257. PLASMA POLYMER COATING TECHNOLOGY FOR ICF TARGETS
$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 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 2 mm diameter capsule target for the National Ignition Facility (NIF). The approach involves first forming a symmetric 2-mm-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.

Keywords: Polymers, Laser Fusion Targets, Plasma Polymer, Ablator

OFFICE OF FOSSIL ENERGY

	FY 2004
OFFICE OF FOSSIL ENERGY - GRAND TOTAL	$12,540,000
OFFICE OF ADVANCED RESEARCH	$12,540,000
ADVANCED RESEARCH MATERIALS PROGRAM	$6,990,000
PROGRAM OVERSIGHT AND COMMUNICATIONS	$480,000
Management of the Advanced Research Materials Program (ORNL-5A)	400,000
Personal Services Contract	20,000
Materials and Components in Fossil Energy Applications Newsletter (MCNL-5)	60,000
NEW ALLOYS	$2,525,000
Materials for Ultra-Supercritical Steam Power Plants (FEAA061)	900,000
Ultra-Supercritical Steam Cycle Turbine Materials (FEAA069)	300,000
Ultra-Supercritical Steam Turbine Materials (ARC-2)	200,000
Evaluation of Advanced Pressure-Boundary Alloys for Heat-recovery Systems (ORNL-2C)	240,000
Development of Oxide Dispersion-Strengthened Alloy for Heat Exchanger Tubing (SMC-2)	100,000
Oxide Dispersion-Strengthened Alloys (ORNL-2E)	230,000
Optimization of Hoop Creep Response in ODS-FECRAL Tubes (UCSD-2)	100,000
Reduction in Defect Content in Oxide Dispersion-Strengthened Alloys (UL-2)	100,000
Testing of a Very High-Temperature Heat Exchanger for IFCC Power Systems (UNDEERC-4)	100,000
Fireside Corrosion of Alloys for USC Plants Environments (ANL-4)	175,000
In-Plant Corrosion Probe Tests of Advanced Austenitic Alloys (FW-5)	80,000
COATINGS	$1,365,000
Extended Alloy Lifetimes Through Improved Coating Performance and Reactive Element Optimization (ORNL-2B)	210,000
Effect of Chromium on Fe/Al Weld-Overlay Coatings for Corrosion Protection (LU-2)	100,000
Yttria-Stabilized Zirconia Thermal Barrier Coatings by MOCVD (ORNL-1A)	225,000
Modeling of Chemical Vapor-Deposited Zirconia for Thermal Barrier and Environmental Barrier Coatings (UOL-3)	110,000
Platinum-Enriched, Two-Phase (g+g'-bond Coating on Ni-based Superalloys (TTU-2)	85,000
Coating Microstructure-Property-Performance Issues (INEL-2)	170,000
Corrosion Resistant Ceramic Coatings (ORNL-1B)	250,000
Development of Nondestructive Evaluation Methods for Ceramic Coatings (ANL-1)	215,000
FUNCTIONAL MATERIALS	$1,500,000
Improved Refractory Materials for Slagging Gasifiers in IGCC Power Systems (ARC-1)	200,000
Use of Carbon Fiber Composite Molecular Sieves for Air Separation (ORNL-3E)	300,000
Development of Inorganic Membranes for Hydrogen Separation (ORNL-3B)	350,000
Palladium-Coated Vanadium-Alloy Membranes for Hydrogen Separation (LANL-3)	100,000
Economic Fabrication of Membrane Materials (ORNL-3H)	200,000
Brazing Technology for Gas-Separation Membranes: the Effect of PD Additions on the Solidus/Liquidus Temperatures and Wetting Properties of Ag/Cuo_x-Based Air Brazes (PNL-3)	350,000

OFFICE OF FOSSIL ENERGY (continued)

	FY 2004
OFFICE OF ADVANCED RESEARCH (continued)	
ADVANCED RESEARCH MATERIALS PROGRAM (continued)	
BREAKTHROUGH ACTIVITIES	$1,120,000
Multi-Phase, High-Temperature Alloys: Exploration of Laves-Phase Strengthening of Steels (ORNL-2D)	110,000
Mo-Si-B Alloy Development (ORNL-2I)	150,000
In-Situ Mechanical Property Measurement, and Influence of Impurity Elements on Grain-Boundary Strength of Cr and Mo Alloys (WVU-2)	100,000
Novel Processing of Mo-Si-B Intermetallics for Improved Efficiency of Power Systems (AMES-2)	150,000
Microstructural Evolution of TiAl-intermetallic Alloys Containing W and B (UT-2A)	100,000
Novel Structures and Properties Through Controlled Oxidation (ORNL-4A)	200,000
Concepts for Smart, Protective, High-Temperature Coatings (ORNL-4C)	120,000
Development of a Commercial Process for the Production of Silicon Carbide Fibrils (REMAXCO-5)	100,000
Advanced Processing of Metallic Powders (AMES-3)	90,000
ADVANCED METALLURGICAL PROCESSES PROGRAM	$5,550,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,000,000
Advanced Foil Lamination Technology	600,000
Advanced Casting Technologies	400,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$4,550,000
Advanced Refractories for Slagging Gasifiers	600,000
Low-Chrome/Chrome Free Refractories for Slagging Gasifiers	400,000
Steam Turbine Materials and Corrosion	300,000
Abrasion and Erosion of Materials for Fossil Energy Systems	250,000
Sensors to Detect Corrosion Under Ash Deposits	1,000,000
Metallic Materials Development for Solid Oxide Fuel Cell Applications	1,100,000
Materials Performance for Heat Exchangers & Other Balance of Plant Components for Solid Oxide Fuel Cells	900,000

OFFICE OF FOSSIL ENERGY

The Office of Fossil Energy's responsibilities include management of the Department's fossil fuels (coal, oil, and natural gas-research and development program. This research is generally directed by the Office of Coal Technology, the Office of Gas and Petroleum Technology, and the Office of Advanced Research and Special Technologies in support of the National Energy Strategy Goals for Increasing Energy Efficiency, Securing Future Energy Supplies, Respecting the Environment, and Fortifying our Foundations. Three specific fossil energy goals are currently being pursued:

1. The first is to secure liquids supply and substitution. This goal targets the enhanced production of domestic petroleum and natural gas, the development of advanced, cost-competitive alternative fuels technology, and the development of coal-based, end-use technology to substitute for oil in applications traditionally fueled by liquid and gaseous fuel forms.

2. The second is to develop power generation options with environmentally superior, high-efficiency technologies for the utility, industrial, and commercial sectors. This goal targets the development of super-clean, high-efficiency power generation technologies.

3. The third is to pursue a global technology strategy to support the increased competitiveness of the U.S. in fossil fuel technologies, to maintain world leadership in our fossil fuel technology base, and provide expanded markets for U.S. fuels and technology. This crosscutting goal is supported by the activities in the above two technology goals.

OFFICE OF ADVANCED RESEARCH

ADVANCED RESEARCH MATERIALS PROGRAM

Fossil Energy materials-related research is conducted under the Advanced Research Materials Program. The goal of the Fossil Energy Advanced Research Materials Program is to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by DOE-FE. The purpose of the Program is to develop the materials of construction, including processing and fabrication methods, and functional materials necessary for those systems. The scope of the Program addresses materials requirements for all fossil energy systems, including materials for coal fuels technologies and for advanced power generation technologies such as coal gasification, heat engines, combustion systems, and fuel cells. The Program is aligned with the development of those technologies that are potential elements of DOE-FE's initiative on clean and efficient power generation from coal, 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: 1) new and improved high-temperature alloys with superior strength and corrosion resistance compared to current alloys available for high-temperature heat exchanger applications, 2) coatings for providing protection to materials needed for service in extreme conditions of high temperature and corrosiveness, including corrosion research to understand the behavior of such materials and coatings in coal-processing environments, 3) 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 4) concepts and approaches for providing materials with properties beyond those available in current materials including, for instance, new combinations of surface properties and durability; and new concepts for strengthening mechanisms for high-temperature alloys to provide higher-temperature capabilities, or combined strength and high-temperature corrosion resistance. 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.

PROGRAM OVERSIGHT AND COMMUNICATIONS

258. MANAGEMENT OF THE ADVANCED RESEARCH MATERIALS PROGRAM (ORNL-5A)
$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 objective of the Advanced Research Materials Program is to conduct long-range research and development that addresses the materials needs of fossil energy systems and ensures the development of advanced materials and processing techniques. The purpose of this task is to provide technical management leadership for the DOE Fossil Energy Advanced Research Materials Program in accordance with procedures approved by DOE.

This task is responsible, in collaboration with DOE-HQ and DOE-NETL, for preparing planning documents, including R&D "road maps." ORNL is responsible for preparing its budget proposals (FWPs) for the program;

recommending work to be accomplished by subcontractors, other federal laboratories, and by ORNL; placing and managing subcontracts for fossil energy materials development at industrial research centers, universities, and other government laboratories; communicating program goals and results to industry and the research and development community; and reporting the progress of the program.

Keywords: Advanced Research Materials, Management

259. 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: R. R. Judkins, 865-574-4572

The task provides funds for a personal services subcontract for services related to the preparation of exhibits for and the management of exhibits at external conferences.

Keywords: Exhibits, Management

260. MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS NEWSLETTER (MCNL-5)
$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

The purpose of this task is to publish a newsletter that communicates current developments, the underlying rationale for materials needs, and planned activities in materials and components in fossil energy applications.

Keywords: Components, Fossil Energy, Newsletter

NEW ALLOYS

261. MATERIALS FOR ULTRA-SUPERCRITICAL STEAM POWER PLANTS (FEAA061)
$900,000
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 research is to fulfill a critical need for materials technology required to design, construct, and operate an ultra-supercritical (USC) steam boiler with much reduced heat rate and increased efficiency. Although several of the advanced materials to be used in such a boiler have been approved for construction under the rules ASME Section I, experience with these materials is lacking in regard to fabrication of components, validity of transient analysis procedures, and specification of corrosion allowances. In addition, for the highest-temperature components, there is interest in the potential of Ni-based alloys with which there is little experience in steam plant. The research undertaken here will provide an essential database to the designers, manufacturers, and users of the USC steam plant.

Keywords: Ultra-Supercritical, Boiler, Alloys

262. ULTRA-SUPERCRITICAL STEAM CYCLE TURBINE MATERIALS (FEAA069)
$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: P. J. Maziasz, 865-574-5081

The objectives of this project are to define the materials challenges confronting the revised steam turbine designs required for operation under ultra-supercritical steam conditions, to prioritize the high-performance materials research needs, and to conduct research to evaluate and qualify new commercial or developmental materials that meet the need for feasibility design and analysis.

Keywords: Ultra-Supercritical, Turbine

263. ULTRA-SUPERCRITICAL STEAM TURBINE MATERIALS (ARC-2)
$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: G. R. Holcomb, 541-967-5874

Ultra-supercritical (USC) steam power plants offer the promise of higher efficiencies and lower emissions. Current goals of the U.S. Department of Energy's Advanced Power Systems Initiatives include coal-fired generation at 60% efficiency, which would require steam temperatures of up to 760˚C. This research examines the steam-side oxidation of advanced alloys for use in USC steam systems, with emphasis placed on alloys for high- and intermediate-pressure turbine sections. To be examined are the effects from steam temperature, steam pressure, and, to a limited extent, the effect of sample curvature. Curved component surfaces can modify the spallation behavior of oxides formed on them by changing the stress fields that are the driving force to detach part or all of the scale. The importance of steam chemistry also is recognized, and will be controlled during supercritical steam exposures. Research in progress from cyclic oxidation in moist air, thermogravimetric analysis in steam, and furnace exposures in moist air.

Alloys examined are of interest for use in USC turbine applications. A subset of the alloys examined by the Advanced Power System Initiative on USC steam boilers, selected for examination for USC turbines, include the ferritic alloy SAVE12, the austenitic alloy SUPER 304H, the high Cr and high Ni alloy HR6W, and three nickel-base superalloys Alloy 617, Alloy 230, and Alloy 740. Also of interest are four superalloys identified as candidates for blade materials for USC conditions: Alloy M-252, Refractory 26, Nimonic 90, and Alloy 718. Two nickel-base alloys, J1 and J5, were produced with low coefficient of thermal expansion for use in solid oxide fuel cells.

Keywords: Ultra-Supercritical, Steam Turbine, Alloys, Superalloys

264. EVALUATION OF ADVANCED PRESSURE-BOUNDARY ALLOYS FOR HEAT-RECOVERY SYSTEMS (ORNL-2C)
$240,000
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. P. Shingledecker, 865-574-5108

The purpose of this task is to evaluate structural alloys for improved performance of high-temperature alloys and components in advanced combined-cycle and coal-combustion systems, with emphasis on cycles at operating temperatures of 700˚C and higher. Emphasis has been transferred from improving austenitic steels to ferritic steels, since these latter alloys comprise a very large part of any fossil-fired steam plant. Any advance in high-temperature properties that allows these alloys to be used above 620˚C (which appears to be the maximum operating temperature of current, ‘advanced’ ferritic steels) would be of significant benefit to the power generation industry.

Keywords: Alloys, Heat Recovery

265. DEVELOPMENT OF OXIDE DISPERSION-STRENGTHENED ALLOY FOR HEAT EXCHANGER TUBING (SMC-2)
$100,000
DOE Contacts: F. M. Glaser, 301-903-2784, V. U. S. Rao, 412-386-4743, M. H. Rawlins, 865-576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, 865-574-4451
Special Metals Corporation Contact: G. Smith, 304-526-5057

This project is intended to generate information and understanding for incorporation into a database being generated by the team assembled by the Edison Welding Institute (EWI) 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 advanced coal combustion and conversion power plant modules. This effort at ORNL has five main objectives: elevated-temperature mechanical testing of joints; extension of a transient liquid-phase bonding technique for use with MA956; evaluation of the effect of joining on high-temperature, oxidation-limited, service life of the tubes; assembly of data required by designers; and review of implications of ODS properties on heat exchanger design. The successful outcome of this (overall) project will result in developments that allow ODS alloys to be used with confidence in a variety of applications previously not possible with metallic materials.

Keywords: Alloys, ODS, Heat Exchanger

266. OXIDE DISPERSION-STRENGTHENED ALLOYS (ORNL-2E)
$230,000
DOE Contacts: F. M. Glaser, 301-903-2784, V. U. S. Rao, 412-386-4743, M. H. Rawlins, 865-576-4507
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’s advanced coal combustion, gasification, and other utilization processes to operate at temperatures higher than are possible with conventionally-strengthened alloys. The original scope of the effort included 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. Following the successful completion of that task, the project was refocused on the needs of the broader range of ferritic ODS-alloys, especially the FeCrAl-based alloys, with the purpose of developing 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. In particular, emphasis has been placed on joining, and on processing modifications to increase the hoop strength of ODS tubes.

The intended output of this project is a compilation of information that facilitates the assessment of the applicability of ODS alloys to the needs of high-temperature equipment required in DOE’s advanced power plants. Efforts to expedite the application of the general class of ODS alloys to meet the needs of advanced fossil-fired power plants (in conjunction with the NETL Combustion and Gasification Product Line teams) are proposed as a route for translating the results of this program into practice.

Keywords: Alloys, ODS, High Temperature

267. OPTIMIZATION OF HOOP CREEP RESPONSE IN ODS-FeCrAl TUBES (UCSD-2)
$100,000
DOE Contacts: F. M. Glaser, 301-903-2784,
V. U. S. Rao, 412-386-4743, M. H. Rawlins,
865-576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, 865-574-4451
University of California at San Diego Contact:
B. K . Kad, 619-534-7059

Oxide dispersion strengthened (ODS) Fe_3Al and Fe-Cr-Al based (MA956) alloys are currently being developed for heat-exchanger tubes for eventual use at operating temperatures of up to 1100°C in the power generation industry. The development challenge is to produce thin-walled tubes, employing powder extrusion methodologies, with a) adequate increased strength for service at operating temperatures to b) mitigate creep failures by enhancing the as-processed grain size via secondary recrystallization. The dispersion distribution is unaltered on a micro scale by recrystallization, but the high aspect ratio grain shape typically obtained limits grain spacing, and consequently the hoop creep response. Improving hoop creep in ODS-alloys requires an understanding and manipulating the factors that control grain alignment and recrystallization behavior. An additional challenge is to preserve this microstructure during subsequent joining operations. This project examines i) efforts to enhance the hoop creep response in (ODS) Fe_3Al and MA956 alloys, and ii) evaluation of non-fusion joining methodologies for symmetrical (or circular) cross-sections as envisaged in heat-exchanger system construction. The performance variance for the two alloys (ODS) Fe_3Al and MA956 has been described in detail with respect to their specific chemistry and processing particulars. Current results indicate a 100% improvement in creep stress threshold for improvised heat-treatments and thermal-mechanical treatments. Such hoop creep improvements can be preserved in selected non-fusion joining techniques.

Keywords: Tubes, ODS, Intermetallics, Alloys, Creep

268. REDUCTION IN DEFECT CONTENT IN OXIDE DISPERSION-STRENGTHENED ALLOYS (UL-2)
$100,000
DOE Contacts: F. M. Glaser, 301-903-2784,
V. U. S. Rao, 412-386-4743, M. H. Rawlins,
865-0576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, 865-574-4451
The University of Liverpool Contact: A.R. Jones,
151-794-8026

The high-temperature creep strength of oxide dispersion-strengthened (ODS) FeCrAl alloys owes much to the development of a suitable grain structure. Existing processing routes may lead to extremely coarse, elongated microstructures which are ideal for creep resistance, and are made possible by the presence of the oxide dispersion and steered by the route taken during the latter stages of production. For example, in extruded tubes a microstructure elongated parallel to the extrusion direction is usual, and has been shown to give enhanced creep performance in applications where the principal stress acts parallel to the elongated grains. In the case of extruded tube intended for use in an internally-pressurized system, however, the principal stress is a hoop stress that acts perpendicular to the direction of grain elongation, thus rendering any advantage due to the microstructure ineffective. It would seem that the ideal microstructure to resist creep in a pressurized tube where there exist hoop and axial stress components would be a helical one.

The feasibility of creating a helical microstructure in ODS FeCrAl tube by plastically twisting the tube prior to final recrystallization is presently underway on a laboratory scale, and also on a quasi-commercial scale. The greatest obstacle to achieving high levels of torsional strain in a tube is that the tube has a tendency to buckle and collapse. During initial torsion trials a number of experimental parameters, such as temperature, strain rate, degree of twist and the use of mandrels, was investigated. Mathematical modeling of tube collapse is also being performed in tandem. Data collected so far are encouraging, and show that a through-wall, helically-orientated grain structure can indeed be created by the techniques investigated. Twisting trials have now moved on to a larger, more commercially-realistic scale, using specialist twisting and heating equipment.

On the other hand, the idea of an optimized microstructure is subjective, and depends upon the intended use of the ODS FeCrAl alloy, and this should be borne in mind when tailoring microstructures to applications. In certain situations, a refined grain structure may be preferable, with finer, more equiaxed grains. The effect on the microstructure of a commercial ODS FeCrAl alloy of the addition of ODS-free material has been investigated. The rationale used was that the ODS-free regions in the alloy should provide sites for rapid recrystallization and, thus, trigger more ready nucleation throughout the alloy. The interaction of these ODS-free regions with the surrounding alloy has been studied by electron microscopy and diffraction techniques.

Keywords: Alloys, ODS, Defects

269. TESTING OF A VERY HIGH-TEMPERATURE HEAT EXCHANGER FOR IFCC POWER SYSTEMS (UNDEERC-4)
$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

Laboratory- and pilot-scale tests of a very high-temperature heat exchanger (HTHX) that could be used to produce pressurized air at up to 2000˚F for an indirectly-fired, combined-cycle (IFCC) power plant were performed, while firing three coal–biomass blends. An IFCC using this type of heat exchanger has the potential to reach efficiencies of 45% when firing coal, and over 50% when a duct burner is used to additionally heat the gas entering the turbine. Because of its high efficiency, an IFCC system is the most appropriate power concept for employing oxygen-enriched combustion in order to make carbon dioxide removal more economical. By staging combustion of coal in such an oxygen-blown system, the need for flue gas recirculation to manage the flame temperature is reduced, and a maximum amount of energy can be channeled to the gas turbine, raising overall plant efficiency. In addition, reducing the volume of flue gas would substantially reduce the required size of the baghouse or electrostatic precipitator, flue gas desulfurization system, and induced- and forced-draft fans, thereby reducing both capital and operating costs. IFCCs have the added benefit of minimizing water usage by dramatically reducing the amount of cooling and makeup water, as compared to a typical pulverized coal (pc) plant, because only half as much steam is produced. Oxygen blowing would also permit the most economical use of a condensing heat exchanger for reclaiming combustion water, even further reducing the amount of outside water necessary for plant operation. After water condensation, only carbon dioxide is left in the gas stream, which can then be used industrially or sequestered, leaving near-zero emissions. If the system is co-fired with coal and biomass, sequestration of the carbon dioxide would create a net atmospheric reduction of the gas. Calculations have shown that the cost of electricity from such a plant is less than that from an emission-less, natural gas-fired, combined cycle if the cost of the gas is above $5.00/MMBtu. The cost of electricity is also similar to that of an emission-less, integrated, gasification combined cycle, but the operation of an IFCC is much better understood since it is essentially the same as current pc-fired systems. Flowing slag corrosion tests have been completed on alloy MA956, an alumina scale-forming, oxide dispersion-strengthened alloy that is a candidate for construction of an HTHX. The tests lasted 100 hours, with the alloy cooled to 1920˚ or 2100˚F and the slag at 2730˚F. No surface recession was measurable after any test, nor was aluminum depletion significant. However, the protective scale was lost in the higher-temperature test with a switchgrass blend because the solidus temperature of the slag was exceeded.

Keywords: High Temperature, Heat Exchanger, Combined Cycle

270. FIRESIDE CORROSION OF ALLOYS FOR USC PLANTS ENVIRONMENTS (ANL-4)
$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

A program on fireside corrosion, in support of ultra supercritical (USC) plants, is being conducted at Argonne National Laboratory to evaluate the performance of several structural alloys in the presence of mixtures of synthetic coal ash, alkali sulfates, and alkali chlorides. Experiments in the present program address the effects of deposit chemistry, temperature, and alloy chemistry on the corrosion response of alloys at temperatures in the range of 650-800˚C. Fe-based materials selected for the study included intermediate-Cr ferritic and high-Cr austenitic alloys. Ni-base alloys selected for the study include Alloys 600, 601, 617, 690, 625, 602CA, 214, 230, 45TM, HR160, 740, and 693. Data were obtained on weight change, scale thickness, internal penetration, microstructural characteristics of corrosion products, mechanical integrity of the scales, and cracking of scales. The intermediate-Cr ferritic steels exhibited catastrophic corrosion at 650˚C in the presence of 150-300 vppm NaCl in the exposure environment. Several approaches have been developed to modify the chemical composition of the surface region of these alloys in order to improve their corrosion resistance in the fireside environment. For Fe-based austenitic alloys, results followed a bell-shaped curve for the relationship of corrosion rates to temperature, with peak rates at ≈725˚C, but the rate itself was dependent on the alloy chemistry. Results have been generated on the fireside corrosion performance of these alloys and on the role of chlorine concentration in simulated ash deposit in corrosion acceleration. Several Fe-based alloys showed acceptable corrosion rates in the sulfate-containing coal-ash environment, but NaCl in the deposit led to catastrophic corrosion at 650 and 800˚C. Ni-based alloys generally exhibited less corrosion than the Fe-base alloys under similar exposure conditions; however, they were susceptible to localized corrosion in the form of pits.

Keywords: Alloys, Corrosion, Ultra-Supercritical

271. IN-PLANT CORROSION PROBE TESTS OF ADVANCED AUSTENITIC ALLOYS (FW-5)
$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: G. Stanko, 973-535-2242

In-plant corrosion probes will be installed in a utility boiler as part of the Phase III Work Scope of the ORNL Project: Fireside Corrosion Testing of Candidate Superheater Tube Alloys, Coatings, and Claddings. Phase I consisted of isothermal laboratory testing of various wrought alloys, coatings, and claddings, whereas in Phase II, air-cooled retractable probes were tested in a 250 MW coal-fired boiler burning high-sulfur coals. The probes were built from materials evaluated in Phase I. In the Phase I and II studies, the corrosion resistance of materials was evaluated at temperatures up to 730˚C (1350˚F). In Phase III, air-cooled probes will be designed to exposed materials in a boiler environment at temperatures up to 1150˚C (2100˚F), primarily to assess the corrosion resistance of candidate materials for the construction of air heaters in advanced-cycle plants. The probes will be fabricated from oxide dispersion-strengthened (ODS) alloys, e.g., MA956, PM2000, and nickel-based superalloys, e.g., 230, 617, 693, and 602CA.

Keywords: Alloys, Austenitic, Corrosion

COATINGS

272. EXTENDED ALLOY LIFETIMES THROUGH IMPROVED COATING PERFORMANCE AND REACTIVE ELEMENT OPTIMIZATION (ORNL-2B)
$210,000
DOE Contacts: F. M. Glaser, 301-903-2784, V. U. S. Rao, 412-386-4743, M. H. Rawlins, 865-576-4507
Oak Ridge National Laboratory Contact: B. A. Pint, 865-576-2897

Conventional Fe-base ferritic and austenitic alloys are readily attacked in steam and exhaust gas environments due to the presence of water vapor and its reaction with normally-protective chromia scales. Alumina scales are not as severely affected by the presence of water vapor. However, the addition of Al to the base alloy generally reduces its high-temperature creep strength. Therefore, the performance of aluminide coatings is being studied in order to better understand their potential benefit. Laboratory testing has initially focused on high-purity, well-controlled coatings made by chemical vapor deposition (CVD) on representative ferritic (Fe-9Cr-1Mo- and austenitic (type 304L stainless steel) substrates. Using an oxidation test with a thermal cycle time of 100h, the coatings have remained protective for over 10,000h at 700˚C and 5,000h at 800˚C in air + 10% water vapor. The uncoated substrates suffer severe oxidation attack in this environment. The effect of temperature and coating thickness is being studied in order to verify a lifetime model that was developed earlier. By testing the coatings to failure, the critical (or minimum) Al content, C_b, needed to provide protection in this environment will be determined. The role of substrate impurities on coating performance also is being investigated. Uncoated alumina-forming alloys also are being investigated in order to better understand the role of minor alloying additions on oxidation lifetime. Generally, lifetime is a function of the starting Al reservoir, C_b, and the rate at which Al is consumed by oxidation, including the effects of scale spallation. Scale growth and spallation are heavily dependent on optimized reactive element-interstitial ratios. As an example, a commonly used Fe-40at%Al composition (containing ZrC precipitates) exhibits a relatively short lifetime during 1h cycles at 1200˚C. However, by increasing the Zr/C ratio or switching to Hf doping, a 2 or 6X increase, respectively, in lifetime was achieved. The 1000˚C yield stresses of these materials were measured to determine if the change in lifetime could be attributed to a change in their mechanical properties. The lifetime of ferritic Fe(Al-alloys also is being optimized. Previous work showed that Hf was very effective in improving the oxidation lifetime of Fe_3Al. However, Y additions were found to be much more effective in improving the lifetime for Fe-18Al. One problem that has been encountered in Y-doped ferritic alloys is the accelerated, alloy grain boundary oxidation, so-called “broccoli” attack, which severely reduces lifetime during some oxidation tests at 1200˚ and 1250˚C. Co-doping with Ti or Hf is being used to reduce this problem, which is associated with grain boundary carbide oxidation. Additions of Cr and Mn in Fe-17Al are being examined in order to extend lifetime by reducing C_b. Finally, internal nitriding has been found to accelerate the oxidation rate of undoped ferritic Fe-19Al-(1-5)Cr alloys at 900˚ in laboratory air. This phenomenon has been previously reported for Fe_3Al and FeAl at 900˚-1200˚C. Additions of Ti, Y, Hf or Zr eliminated the problem, while 2-5%Ni additions showed no benefit. This problem is a concern for aluminide coatings, but no acceleration was observed at 700˚ or 800˚C in air.

Keywords: Alloys, Coatings, Lifetime

273. EFFECT OF CHROMIUM ON Fe/Al WELD-OVERLAY COATINGS FOR CORROSION PROTECTION (LU-2)
$100,000
DOE Contacts: F. M. Glaser, 301-903-2784, V. U. S. Rao, 412-386-4743, M. H. Rawlins, 865-576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, 865-574-4451
Lehigh University Contact: J. N. DuPont and A. R. Marder, 610-758-4197

Fe-Al-Cr-based alloys exhibit outstanding resistance to high-temperature corrosion in sulfidizing environments. In this project, alloy compositions are being optimized to allow their application as weld-overlay coatings in fossil-fired boilers. Several cast alloys representative of weldable Fe-Al-Cr weld overlay coating compositions were exposed to a mixed oxidizing/sulfidizing gaseous environment (10%CO- 5%CO_2- 2%H_2O- 0.12%H_2S- N_2). The FeAlCr alloys (Fe-12.5Al, Fe-10Al-5Cr, and Fe-7.5Al-10Cr-were compared to a currently-used Ni-based weld overlay coupon of Alloy 622. Samples were held at 500C for 100 - 2000 hours. It was found that the corrosion kinetics for all three of the Fe-Al-Cr alloys were significantly lower than the corrosion kinetics of Alloy 622. For example, during 2000 hours of exposure to the corrosive environment, Alloy 622 gained approximately 20 mg/cm^2 whereas all three of the FeAlCr alloys gained less than 0.5 mg/cm^2. Corrosion scale morphology was also considered and it was found that Alloy 622 formed a thick, porous scale rich in nickel and sulfur, whereas the FeAlCr alloys formed small, block-like nodules that were rich in iron and sulfur. It was concluded that several of the weldable FeAlCr overlay coating compositions could be deposited crack-free, and can provide superior, high-temperature corrosion protection than Alloy 622.

Weld-overlay coatings were also characterized to determine if the weld microstructure had any effect on the cracking behavior of the welds. X-ray diffraction (XRD) was used to identify the phases present within the weld overlay coatings. It was found that welds containing <6wt%Cr formed intermetallic phases (Fe_3Al and/or FeAl) above approximately 11wt%Al. All alloys containing less than approximately 4wt%Cr formed $(Fe,Al)_3C$ carbides, which were identified using XRD. Alloys containing chromium additions greater than approximately 6wt%Cr showed only ferrite to be present, although weak Cr-rich carbide peaks were observed in these samples as well. Light optical microscopy (LOM) was also used to make observations about the weld microstructure. LOM observations of weld samples confirmed the existence of highly-acicular carbides in welds containing lower chromium concentrations [$(Fe,Al)_3C$], and small, spherical carbides in samples containing high chromium concentrations (Cr-rich carbides). The intermetallic phases cannot be observed using LOM, so that the presence of this phase was not considered in the LOM observations.

Keywords: Weld Overlay, Coatings, Oxidation

274. YTTRIA-STABILIZED ZIRCONIA THERMAL BARRIER COATINGS BY MOCVD (ORNL-1A)
$225,000
DOE Contacts: F. M. Glaser, 301-903-2784, V. U. S. Rao, 412-386-4743, M. H. Rawlins, 865-576-4507
Oak Ridge National Laboratory Contact: T. M. Besmann, 865-574-6852

Yttria-stabilized zirconia (YSZ) is used as a thermal barrier coating (TBC) to protect superalloy components used in gas turbines, such as blades and vanes. The current method for YSZ fabrication for TBC applications is by air-plasma spraying (APS) or electron beam physical vapor deposition (EB-PVD). APS gives reasonable deposition rates, but has a limited life due to aging effects as a result of its porous and lamellar structure. The EB-PVD coatings are more stable, accommodating thermomechanical stresses via their characteristic strain-tolerant, columnar microstructure. EB-PVD and APS, however, are primarily line-of-sight techniques, which often leaves “hidden areas” uncoated. EB-PVD processing also has low throughput, and high capital cost. The process of metal-organic chemical vapor deposition (MOCVD) is currently being investigated as an economical alternative to EB-PVD and APS, with the potential for better overall coverage as well as the ability to produce thick ($\geq$250 μm), strain-tolerant, columnar coatings. The current metal-organic chemical vapor deposition (MOCVD) process utilizes a cold wall reactor with liquid delivery of a metal-organic precursor solution to deposit YSZ. Thick thermal barrier coatings with a columnar structure have been successfully deposited on developmental FeCrAlY material. TBC coupons were tested under thermal cycling and resisted spallation through 1000 cycles of 1 hour to a temperature of 1100˚C when the deposit was on a pre-oxidized surface. The current MOCVD system is being scaled-up to deposit coatings on prototypical turbine blade width sections. Through utilization of fluid dynamics modeling coupled with kinetic behavior, an efficient deposition system has been designed. Components have been constructed and operational testing is beginning. One of the scale-up issues has been adequate and accurate delivery of precursor solution to a vaporization system, and this has been solved through installation of a continuous, non-pulsating liquid delivery pump. Interactions with Pratt & Whitney have resulted in an informal agreement on testing prototype YSZ coatings. Pratt & Whitney will be supplying standard burner rig test substrates for coating at ORNL. These will be then provided to Pratt & Whitney for burner rig testing. Samples will be shared for evaluation.

Keywords: YSZ, MOCVD, Thermal Barrier Coatings

275. MODELING OF CHEMICAL VAPOR-DEPOSITED ZIRCONIA FOR THERMAL BARRIER AND ENVIRONMENTAL BARRIER COATINGS (UOL-3)
$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 Contact: I. G. Wright, 865-574-4451
University of Louisville Contact: T. L. Starr, 502-852-1073

Yttria-stabilized zirconia (YSZ) coatings can provide effective thermal and environmental protection for advanced energy systems. A chemical vapor deposition (CVD) method for these coatings offers advantages over currently-available application methods. Critical requirements for a successful CVD process are high coating deposition rate and uniform coating thickness on components of size and geometry typical of advanced turbine systems. A computer model has been developed to simulate the direct liquid injection CVD process, using mixed zirconium and yttrium alkoxide precursors. Previous results using this model provide understanding of the mass transport and reaction kinetics that control coating deposition. A coupon-scale reactor demonstrated uniform coating at rates up to 50 µm/hr. Current research efforts use the process model to design and evaluate options for a subscale reactor that is under development at Oak Ridge National Laboratory. A subscale reactor must demonstrate uniform, high-rate deposition on both sides of a 10-12 cm substrate. This configuration and dimension is comparable to the cross-flow dimension in a full-scale gas turbine blade. The computer model is used to evaluate design options for holding and heating the substrate and for introducing the precursor vapor. Methods developed with the subscale reactor should be transferable to future design of a full-scale turbine blade coating system. Three basic approaches are considered: impinging flow, parallel flow and pulse. The impinging flow reactor is most comparable to the previous coupon-scale process. Modeling results for various inlet and outlet configurations show that uniform coating can be achieved only with a mid-process switch in outlet configuration. In addition to the complexity added by this mid-process switch, this configuration would be difficult to implement for a full-scale coating system. The parallel flow configuration also provides uniform coating thickness. No mid-process switch is needed; however the geometry of the deposition chamber is critical. A full-scale coating system would include internal baffles to guide the convective flow that controls deposition uniformity. The pulse deposition approach involves periodic filling and evacuation of the coating chamber. Initial modeling results suggest that uniform deposition is possible with this method. Scale-up feasibility is a trade-off between the complexity of the cyclic, filling-evacuation process, and the potential simplicity of the overall deposition chamber. Overall, these modeling results support the feasibility of a direct liquid injection CVD process for deposition of thermal and environmental barrier coatings on advanced energy system components.

Keywords: Thermal Barrier Coatings, Modeling, Zirconia, CVD

276. PLATINUM-ENRICHED, TWO-PHASE (g+g'-BOND COATING ON Ni-BASED SUPERALLOYS (TTU-2)
$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: Y. Zhang, 931-372-3186

A metallic bond coating is an essential feature of the thermal barrier coatings required on hot gas path components in gas turbines. This project is aimed at increasing the lifetime of such coatings by increasing the inherent oxidation resistance of the metallic bond coating, while also reducing its tendency for interaction with the alloy substrate. A Pt-enriched g+g' two-phase coating was applied to directionally-solidified Ni-based superalloy René 142 substrates with three different Hf levels (0.02, 0.76, and 1.37 wt.%). The coating was prepared by electroplating a thin layer of Pt (~7 µm) on the superalloy followed by a diffusion treatment of 2h in vacuum at 1150˚C. The as-deposited coating exhibited a g+g' two-phase microstructure with a major composition of Ni-16Al-18Pt-7Cr-9Co (in at.%) along with some incorporation of refractory elements from the substrates. Cyclic oxidation tests at 1100˚C in air indicated improved oxidation resistance of the René 142 alloys with the Pt-enriched g+g' coatings. In addition, the oxidation resistance of both uncoated and coated alloys was proportional to the Hf content in the substrate. Compared with the single-phase coating, slightly higher mass gain and localized spallation were observed on the g+g' two-phase coating, which might be due to the segregation of refractory elements and high sulfur levels in these superalloy substrates.

Keywords: Superalloys, Coatings, Pt-Enriched

277. COATING MICROSTRUCTURE-PROPERTY-PERFORMANCE ISSUES (INEL-2)
$170,000
DOE Contacts: F. M. Glaser, 301-903-2784, V. U. S. Rao, 412-386-4743, M. H. Rawlins, 865-576-4507
Oak Ridge National Laboratory Contact: I. G. Wright, 865-574-4451
Idaho National Engineering and Environmental Laboratory Contact: R. N. Wright, 208-526-6127

This study focuses on the relationships between spray parameters and performance of thermally-sprayed intermetallic coatings for high-temperature oxidation and corrosion resistance. Coating performance is being assessed by corrosion testing of free-standing coatings, thermal cycling of coating substrates, and coating ductility measurement. Coating corrosion resistance was measured in a simulated coal combustion gas environment (N_2-CO-CO_2-H_2O-H_2S) at temperatures from 500 to 800˚C using thermo-gravimetric analysis (TGA). TGA testing was also performed on a typical ferritic-martensitic steel, austenitic stainless steel, and a wrought Fe_3Al-based alloy for direct comparison to coating behavior. FeAl and Fe_3Al coatings showed corrosion rates slightly greater than that of wrought Fe_3Al, but markedly lower than the steels at all temperatures. The corrosion rates of the coatings were relatively independent of temperature. Thermal cycling was performed on coated 316SS and nickel alloy 600 substrates from room temperature to 800˚C to assess the relative effects of coating microstructure, residual stress, and thermal expansion mismatch on coating cracking by thermal fatigue. Measurement of coating ductility was made by acoustic emission monitoring of coated 316SS tensile specimens during loading.

Keywords: Intermetallics, Coatings, Microstructure

278. CORROSION RESISTANT CERAMIC COATINGS (ORNL-1B)
$250,000
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 useful operating life of the materials used in fossil energy conversion and combustion systems is highly dependent on the operating temperatures, the variability of the feed stock, and the rate of throughput, all of which are dictated by economic susceptibility to corrosion by molten slags, alkali metals, and gases in these harsh operating environments. Therefore, in order to utilize the attractive properties of ceramic materials and extend their service lifetimes, additional measures must be employed to protect the materials from these corrosive environments. To address this issue, the development of novel coatings utilizing low-cost aqueous processing methods (such as dip coating) is being pursued. Colloidal processing of ceramic particles in aqueous suspension offers an economic route for forming uniform, thick ceramic coatings on complex-shaped components via a simple process. Application of the ORNL dip coating process was examined for depositing mullite coatings on sintered alpha silicon carbide substrates, and the ARC-developed chromia system on chromia refractory bricks.

Keywords: Ceramics, Coatings, Corrosion

279. DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS FOR CERAMIC COATINGS (ANL-1)
$215,000
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

Nondestructive evaluation (NDE) technologies are being developed as non-contact, remote sensing methods for determining the condition or “health” of high temperature ceramic coatings used to protect components in the hot-gas path of advanced, low-emission, high-efficiency gas turbines. The ceramic coatings presently under study include yttria-stabilized zirconia (YSZ) for metal vanes, blades, and combustor liners, and several compositions of environmental barrier coatings (EBCs) for advanced ceramic matrix composites. While such coatings have not been developed for hydrogen-fueled turbines such as those for the FutureGen program, it is likely that similar coatings would be required and similar NDE technologies would be useful. The TBC effort is a task within the recently-established Memorandum of Understanding between the United Kingdom and the United States for collaboration on Fossil Energy Materials.

The primary NDE technologies being developed at Argonne for high-temperature ceramic coatings involve laser-based methods. One method, elastic optical back-scatter (EOBS), has been awarded three patents. The second and more recently developed laser-based method is called Optical Coherence Tomography (OCT). Correlations between EOBS data and the condition of these coatings are developed through cooperative efforts with industry and academia. Partners involved in active cooperation on TBCs include : The University of Pittsburgh, Praxair Surface Technologies located in Indianapolis, IN, and DLR (The German Aerospace Institute) in Koln, Germany. Work related to EBCs is being done in cooperation with Siemens-Westinghouse Power Corporation (SWPC) and ATK-COI ceramics in San Diego, CA. Work on EBCs for SiC is being done in cooperation with NASA-Glenn Research Center. In the work on TBCs, test specimens are provided with various substrate materials, bond coats, surface preparation, controlled thermal cycles (temperature, duration and number of cycles), and coating thickness. Several new test samples were prepared using both electron-beam physical vapor deposition (EB-PVD) and air plasma spray (APS). Additional correlations were established between the EOBS data and number of cycles before spallation. The predictions were within a few 10's of cycles. Analysis of the EOBS data using digital image analysis continues to suggest a strong correlation exists between EOBS data and the topography at the TBC/bond coat interface. This finding is important as several theories directed toward understanding the pre-spall condition suggest that the topography at the interface between the thermally grown oxide layer and the bond coat changes significantly as a function of the number of thermal cycles. The analytical model described last year for analysis of the EOBS was more extensively studied this year. The software package is a "field-solver" for Maxwell's equations and allows prediction of EOBS patterns as a function of various features including the topography of the interface of the thermally-grown oxide (TGO)/bond coat, input laser power, polarization angles, and effect of wavelength. Initial models show a direct prediction of scatter patterns for a "V" notch below the TGO layer with a 75μm EB-PVD coating. The single "V" notch represents one "peg" in the topographical pattern. The OCT system described last year was modified with the addition of new electronics, new laser and better fiber optics. Tests were run on both EBCs and TBCs. This technology has now been demonstrated to allow a direct measurement of thickness of the TBC as well as EBCs. Direct measurement of the thickness of the TGO is possible, but spatial resolution limits in the vertical direction limit the data at the moment.

Keywords: Non-Destructive Evaluation, Ceramics, Coatings

FUNCTIONAL MATERIALS

280. IMPROVED REFRACTORY MATERIALS FOR SLAGGING GASIFIERS IN IGCC POWER SYSTEMS (ARC-1)
$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: J. Bennett, 541-967-5873

Gasifiers are the heart of integrated, gasification, combined-cycle (IGCC) power systems currently being developed as part of the DOE's advanced, coal-fired power plant initiatives, including FutureGen. A gasification chamber is a high-pressure/high-temperature reaction vessel used to contain a mixture of O_2, H_2O, and coal (or other carbon-containing materials) while it is converted into thermal energy and chemicals (H_2, CO, and CH_4). IGCC systems are expected to play a dominant role in meeting the Nation's future energy needs. Gasifiers are also used to produce chemicals that serve as feedstock for other industrial processes, and are considered a potential source of H_2 in applications such as fuel cells. A distinct advantage of gasifiers is their ability to meet or exceed current and anticipated future environmental emission regulations. Also, because gasification systems are part of a closed circuit, gasifiers are considered process-ready to capture CO_2 emissions for reuse or processing, should that become necessary or economically feasible in the future.

The service life of refractory liners for gasifiers has been identified by users as a critical barrier to IGCC system economics and to gasifier reliability and on-line availability. The refractory lining contains the harsh, high-temperature/pressure gaseous environment, an environment that includes molten slag originating from impurities in the carbon source. The molten slag flows over the refractory surface and penetrates it, causing refractory dissolution in the slag, and setting up the environment for refractory spalling to occur, the two primary wear mechanisms of refractories. The current generation of refractory liners need to be replaced after 3 to 24 months of service because of these wear mechanisms. Slag wear of a refractory lining by dissolution is highly dependent on gasifier carbon feedstock, material throughput, gasification temperature, downtime frequency, and system maintenance. Spalling wear of a refractory is influenced by slag penetration depth, gasifier cycling, and rapid temperature changes, and leads to small portions of a liner peeling from the working face lining. Predicting when a refractory lining needs replacement is difficult, and the cost of replacing all or part of the lining exceeds $1M, depending on the extent of the necessary repair/replacement. Compounding material and installation costs are lost opportunity costs that occur when a gasifier is off-line for refractory replacement or repair. Industry would like to have refractory materials that have a predictable and improved service life of 50 pct. ARC's program goal is to attain improved service life and reliability in refractory liners through materials research.

To improve refractory service life, ARC scientists have developed and patented a high chrome oxide, phosphate-containing, refractory composition. This material has exhibited excellent slag penetration resistance properties in laboratory testing, was commercially produced by a refractory manufacturer, has been installed in a commercial coal slagging gasifier, and is undergoing field trials. An expansion of field trials is underway through discussions with several gasifier operators. Because of large variations in gasifier operation and carbon feedstocks, testing of the phosphate-containing refractory material is planned in systems using petroleum coke and coal/petroleum coke carbon feedstock. These plant trials will indicate if a service life improvement occurs in the newly-developed material, or if further modifications of the composition are needed.

Research is also underway at ARC to develop no-chrome or low-chrome oxide refractory materials, refractories not actively considered for gasifier use since the mid 70's to 80's, when early research indicated high-chrome oxide materials had superior performance to all other refractory materials tested. Since that time, significant improvements in refractory technology, new raw materials, and a greater understanding of gasifier wear mechanisms, may make it possible to engineer better no- or low-chrome oxide liner materials. Some driving forces for this research are because chrome oxide refractories: a) have not met the service life requirements, b) have high cost, c) have high density (creating weight, size and joint issues), d) have possible long-term supply issues, e) have perceived/real safety concerns, and f) have limited repair options with lengthy repair turnaround. ARC is researching new materials that include Al_2O_3, MgO, ZrO_2, MgO/Al_2O_3 spinels, or engineered combinations of them, for potential use as hot-face liners.

Keywords: Refractories, Gasifiers, Combined Cycle

281. USE OF CARBON FIBER COMPOSITE MOLECULAR SIEVES FOR AIR SEPARATION (ORNL-3E)
$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:
F. S. Baker, 865-241-1127

The adsorption of oxygen, nitrogen, and carbon dioxide on a carbon fiber composite material was investigated using static and dynamic techniques. Molecular sieving effects in the composite were highlighted by the adsorption of carbon dioxide, a more sensitive probe molecule for the presence of microporosity in adsorbents. The kinetic studies revealed that oxygen was more rapidly adsorbed on the composite than nitrogen, and with higher uptake under equilibrium conditions. Preliminary experiments indicated that the carbon fiber composite is capable of separating oxygen and nitrogen from air on the basis of the different diffusion rates of the two molecules in the micropore network of the composite. It is proposed that a fast-cycle air separation process that exploits a kinetic separation of O_2 and N_2 is feasible using a carbon fiber carbon molecular sieve (CFCMS) composite coupled with electrical swing adsorption (ESA).

To define the micropore size distribution required to obtain effective separation of O_2 and N_2, a series of isotropic pitch-based, activated-carbon fiber products was prepared in which the degree of thermal activation of the carbon fiber was varied in the range of 5-30% (carbon burn-off level). Nitrogen (at 77 K) and CO_2 (at 273 K) adsorption isotherms were determined to characterize the surface area and pore size distribution of the activated carbon fiber products (through application of the density functional theory, DFT, approach). Dynamic measurements were made of the rate of O_2 and N_2 adsorption, respectively, on these products at 294 K over the pressure range of 0.001-0.1 MPa. Activated carbon fibers were also produced from Kraft lignin, a precursor that is known to produce highly-microporous activated carbon products. In response to enquires from several potential users of CFCMS materials, attention was turned to the development of a viable, continuous process for the commercial production of CFCMS material. Similarly, to address engineering issues, preliminary measurements were made to characterize the pressure drop of CFCMS as a function of carbon fiber properties and monolith density.

Keywords: Carbon Fiber, Composite, Molecular Sieve

282. DEVELOPMENT OF INORGANIC MEMBRANES FOR HYDROGEN SEPARATION (ORNL-3B)
$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

Coal gasification offers one of the most versatile and cleanest ways to convert the heating value of coal into electricity, hydrogen, and other energy forms. Rather than burning coal directly, gasification breaks down coal—or virtually any carbon-based feedstock—into its basic chemical constituents. In a modern gasifier, coal is typically exposed to hot steam and carefully controlled amounts of air or oxygen under high temperatures and pressures. Under these conditions, carbon in coal breaks apart, setting into motion chemical reactions that typically produce a mixture of carbon monoxide, hydrogen and other gaseous compounds. An important goal of the Energy Department's coal gasification program is to develop inexpensive membranes, which can selectively remove hydrogen from synthesis gas, so that it can be used as a fuel for future fuel cells, or for refineries or, perhaps one day, as a substitute for gasoline in a hydrogen-powered automobile. Advances have been made recently at the Oak Ridge National Laboratory in the development of microporous inorganic membranes for high-temperature hydrogen separation. Research emphasis during the last year has been directed toward the development of high permeance (high flux), and high separation factor metal-supported membranes.

Keywords: Membranes, Hydrogen Separation

283. PALLADIUM-COATED VANADIUM-ALLOY MEMBRANES FOR HYDROGEN SEPARATION (LANL-3)
$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:
S. N. Paglieri, 505-667-5868

Hydrogen-separating membranes have the potential to facilitate the generation of pure hydrogen for use in fuel cells. Foils of VTi_5, $VCu_{1\text{-}10}$ (atomic %) and Ta coated with thin films of Pd or Pd alloys (Pd–Cu or Pd–Ag), and other metal interlayers were fabricated and tested for hydrogen permeability and stability during operation at temperatures from 320-450ºC. Vanadium-alloy or Ta foils were ion-milled, and coatings between 30 and 250 nm thick were applied to both sides *in-situ*, via electron beam evaporation PVD. Membranes were between 40 and 120 microns thick, and were completely permselective for hydrogen. Pt or Ni surface coatings on VTi_5 foils reduced the permeability by at least an order of magnitude, while a membrane coated with the thinnest Pd layer, 30 nm-exhibited the fastest hydrogen flux decline at 450ºC. Foils of Ta were coated with layers of Ti or Mo and then Pd in order to increase the hydrogen flux stability during operation above 400ºC. Although the hydrogen flux through the coated Ta foils was generally an order of magnitude less than through the V-alloy membranes, the hydrogen flux stability was greater. Composite membranes comprised of porous stainless steel tubes coated with V-Cu alloy and Pd were also fabricated and tested.

The hydrogen flux through a 75 micron thick $Pd/VCu_{1.1}/Pd$ composite membrane with 100 nm Pd per side was 0.66 mol (STP)/m^2·s at 350ºC, and its trans-membrane pressure differential was 3.5 atm (compared to 0.44 mol (STP)/m^2·s for a 71 micron thick $Pd/VCu_{10}/Pd$ membrane at the same conditions). A 50% decrease in hydrogen flux was observed through the $Pd/VCu_{10}/Pd$ membrane after 75 hours at 450ºC. Metallic interdiffusion between various surface coatings and foils tested at different temperatures was characterized by means of AES depth profiles. One mechanism of hydrogen flux decline at 450ºC was found to be diffusion of V to the surface of the Pd coating.

Keywords: Alloys, Membranes, Hydrogen Separation

284. ECONOMIC FABRICATION OF MEMBRANE MATERIALS (ORNL-3H)
$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. R. Armstrong, 865-574-7996

The current class of ceramic monolithic oxygen and hydrogen membranes has relatively low flux, due to high membrane thickness (> 100 µm). In order to reduce the footprint of the separation device, while increasing flux, thinner membranes are required. Thin membranes, however, maybe too fragile to function as self-supported structures in high pressure, fossil environments. As a result, porous supports are used to impart the necessary mechanical behavior, while also allowing for fluid flow through the pore network to the membrane.
In order to use inorganic membranes in a wide array of energy applications, low-cost fabrication methods must be developed that utilize inexpensive membrane and support materials. Calcium ferrite-based ceramics with the Brownmillerite structure recently have been identified as excellent candidates for dense, asymmetric oxygen-transport membranes. The base composition ($Ca_2Fe_2O_5$) elicits strong, mixed conducting behavior, and is easily doped, e.g., with Ga, Al, Cr, Co, Ti, and Ni, to improve the conductivity (via an oxygen vacancy diffusion mechanism) and mechanical stability. Furthermore, metallic supports with high-temperature capabilities (1300˚C) have great potential for improved mechanical strength and reduced material costs.

Keywords: Membranes, Fabrication

285. BRAZING TECHNOLOGY FOR GAS-SEPARATION MEMBRANES: THE EFFECT OF Pd ADDITIONS ON THE SOLIDUS/LIQUIDUS TEMPERATURES AND WETTING PROPERTIES OF Ag/CuO_x-BASED AIR BRAZES (PNL-3)
$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
Pacific Northwest National Laboratory Contact:
S. K. Weil, 509-375-6796

Over the past several years, we have been developing a new method of ceramic-ceramic and ceramic-metal joining, referred to as air brazing. The novelty of the technique is that it can be used to form a predominantly metallic joint directly in air, without need of an inert cover gas or the use of surface reactive fluxes, offering a distinct advantage in bonding the membranes employed in high-temperature electrochemical devices. The resulting bond is hermetic, offers excellent room-temperature strength, and is inherently resistant to oxidation at high temperature. The key to developing a successful filler metal composition for air brazing is to identify a metal oxide wetting agent that is mutually soluble in a molten noble metal solvent. One particular oxide-metal combination that appears readily suited for this purpose is CuO_x-Ag, a system originally of interest in the development of silver-clad, cuprate-based superconductors. Studies of the equilibrium phases studies in this system indicate that there are two invariant points in the pseudobinary CuO_x-Ag phase diagram around which new braze compositions could be developed: 1) a monotectic reaction at 969±1˚C, where CuO and a Ag-rich liquid L_1 coexist with a second CuO_x-rich liquid phase L_2 at a composition of $x_{Ag}/(x_{Ag} + x_{Cu})$= 0.10±0.03 Ag, and 2) a eutectic reaction at 942±1˚C, where CuO and Ag coexist with L_1 at a composition of $x_{Ag}/(x_{Ag} + x_{Cu})$= 0.99±0.005 [*J. Am. Ceram. Soc.*, 81(1998-2181].

In a series of sessile drop experiments conducted under inert atmosphere, Meier et al. demonstrated that the addition of copper oxide to molten silver greatly reduces the contact angle formed between this liquid and a solid alumina substrate [*J. Mater. Sci.*, 30(1995)4781]. The improvement in wetting was speculated to result from: 1-an increase in the oxygen activity of the melt, and 2-the formation of an interfacial compound, $CuAlO_2$. Schüler et al. were the first to recognize that the CuO_x-Ag system could be exploited to bond ceramics directly in air, and demonstrated this by joining blocks of alumina with a 1mol% CuO-Ag braze composition [*J. Mater. Sci: Mater. in Elect.*, 11(200)389]. More recently, our work has focused on investigating the use of CuO_x-Ag-based air brazes as a means of hermetically sealing solid-state electrochemical devices such as hydrogen and oxygen separators.

Because the high-temperature application of the CuO_x-Ag brazes is ultimately limited by the eutectic transformation present in this system, we sought to extend the use temperature by adding a higher melting-point, noble metal element; in this case palladium. We have previously observed that the addition of palladium to the Cu-O-Ag system increases both the liquidus and solidus temperatures, but have not attempted a more detailed study of this phenomenon until now. In the present study, we examine the effect of major and minor compositional deviations on the formation of equilibrium solid and liquid phases in the pseudobinary CuO_x-Ag system. Phase equilibria were determined experimentally, using differential scanning calorimetry, microstructural analysis, and X-ray diffraction. Small additions of palladium were generally found to increase the temperature of the eutectic reaction present in the pseudo-binary system, but to have little effect on a higher-temperature monotectic reaction. However once enough palladium was added (~5 mol%) to increase the new eutectic temperature to that of the original pseudo-binary monotectic reaction, the pseudo-ternary monotectic temperature correspondingly began to move upward as well. The addition of palladium also forced the eutectic point to slightly lower silver concentrations, again causing a convergence with the former monotectic line.

Keywords: Membranes, Gas Separation, Brazing

BREAKTHROUGH ACTIVITIES

286. MULTI-PHASE, HIGH-TEMPERATURE ALLOYS: EXPLORATION OF LAVES-PHASE STRENGTHENING OF STEELS (ORNL-2D)
$110,000
DOE Contacts: F. M. Glaser, 301-903-2784,
V. U. S. Rao, 412-386-4743, M. H. Rawlins,
865-576-4507
Oak Ridge National Laboratory Contacts:
M. P. Brady, 865-574-5153

Exploratory efforts were initiated for alloy design of advanced ferritic and austenitic alloys strengthened by (1) solid solutes, (2) carbide precipitates (MC), and, (3) Laves and other intermetallic phase precipitates. The ultimate goal is to extend the upper temperature limits of these classes of alloys, while co-optimizing oxidation/corrosion resistance. This year, the focus of the work was in assessing strengthening potential via control of Laves-phase precipitates, and to do so in Al-modified compositions capable of exhibiting improved environmental resistance over that of existing Cr_2O_3-forming steels. A series of alloys based on Fe-(10-20)Cr-(10-25)Ni (at.%) was cast and processed by forging and/or heat treating. Alloying additions such as Al, Mo, Nb, and W were evaluated. Emphasis was placed on understanding and manipulation of composition/processing conditions to yield Fe_2Nb base Laves phase precipitates, NiAl precipitates, and MC carbides. Microstructural details as a function of qualitative compositional variables, and preliminary tensile and creep strength data were generated. Oxidation studies from 700-800°C in air and air + 10% water vapor have emphasized the behavior with relatively low additions of Al (< 3 wt.%).

Keywords: Alloys, High Temperature, Oxidation

287. Mo-Si-B ALLOY DEVELOPMENT (ORNL-2I)
$150,000
DOE Contacts: F. M. Glaser, 301-903-2784,
V. U. S. Rao, 412-386-4743, M. H. Rawlins,
865-576-4507
Oak Ridge National Laboratory Contact:
J. H. Schneibel, 865-574-4644

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 DOE-FE's goals for fossil-fired power plants, one of which is to significantly reduce greenhouse emissions. The effort focuses on Mo phase-toughened Mo-Si-B alloys. While very significant progress has been made with Mo-Si-B alloys, a point has now been reached at which industrial-scale processing would be needed for further study of the applications of these alloys. Industrial scale processing has not yet reached the point at which substantial quantities of high-quality material are available. It is therefore planned to gradually transition this effort to the study of novel precipitation-hardened steels.

Keywords: Alloys, Mo-Si-B, Corrosion

288. IN-SITU MECHANICAL PROPERTY MEASUREMENT, AND INFLUENCE OF IMPURITY ELEMENTS ON GRAIN-BOUNDARY STRENGTH OF Cr AND Mo ALLOYS (WVU-2)
$100,000
DOE Contacts: F. M. Glaser, 301-903-2784,
V. U. S. Rao, 412-386-4743, M. H. Rawlins,
865-576-4507
Oak Ridge National Laboratory Contact:
I. G. Wright, 865-574-4451
West Virginia University Contact: B. S. Kang,
304-293-3423

This research is (i) to conduct atomistic computational modeling and simulations on the influence of carbon and oxygen to grain-boundary strength and interfacial fracture of molybdenum alloys, and (ii) to apply and further develop of a transparent indenter measurement (TIM) system for in-situ material mechanical property measurement of selected metallic alloys relevant to the Fossil Energy Materials Program. Segregated near the grain boundaries, impurity elements such as O, N and S, can have important effects on the mechanical properties of hosting structural materials. To minimize the detrimental effects, dispersions (MgO for Cr) or other impurities (C for Mo) are included to alter the microstructures, sometimes resulting in improved ductility. However, the fundamental mechanism is not clear, and the relationship between the features in the microstructure and the ductility enhancement is not robust. For example, although the inclusion of TiO_2 and La_2O_3 dispersions in Cr displays similar microstructure patterns as does MgO, the ductility is not correspondingly improved. We therefore believe a more fundamental mechanism at the atomic scale will provide insightful information. Using FP-LMTO techniques, we carried out a number of numerical simulations to probe the changes in electronic structures and chemical bonding properties due to the complex interactions among the impurity elements and the hosting metal or metal-oxide interface. We have seen interesting features in the charge distribution plot, which may link to ductility enhancement. Such correlations can help to better understand the mechanism and predict the optimal composition for additives. For the second task, a new in-situ TIM system was developed for material mechanical property evaluation, based on a spherical indentation technique. During the indentation process, the in-situ measurement of out-of-plane deformation was carried out, using an integrated, phase-shifting Twyman-Green interferometer. Based on elastic recovery theories and 2D finite element analyses, a procedure was developed to determine the material Young's modulus, using the measured out-of-plane deformation. During loading, the contact radius of spherical indentation was continuously measured, and used to estimate the material's post-yielding true stress-strain curve, using Tabor's empirical relation. An experimental TIM apparatus was assembled, and preliminary tests were conducted on several engineering materials. The results showed good agreement with known material properties.

Keywords: Alloys, Molybdenum, Chromium, Mechanical Properties

289. NOVEL PROCESSING OF Mo-Si-B INTERMETALLICS FOR IMPROVED EFFICIENCY OF POWER SYSTEMS (AMES-2)
$150,000
DOE Contacts: F. M. Glaser, 301-903-2784,
V. U. S. Rao, 412-386-4743, M. H. Rawlins,
865-576-4507
Oak Ridge National Laboratory Contact:
J. H. Schneibel, 865-574-4644
Ames Laboratory Contact: M.J. Kramer.
515-294-0276

Bcc-Mo-based Mo-Si-B alloys have promising high-temperature mechanical properties. In particular, the bcc-Mo+T2(Mo_5SiB_2)-based alloys have excellent resistance to fracture, with toughness values approaching 20 MPa·m^{½} for a continuous a-Mo matrix material. However, a fundamental limitation of these alloys is their poor oxidation resistance at temperatures envisioned for advanced power system goals. On the other hand, the oxidation-resistance of T1 ($Mo_5Si_3B_x$)-based alloys is exceptional, and a consensus is emerging to protect the bcc-Mo-based alloys with an oxidation resistant coating such as the T1-based alloy. The present work explored coating strategies to protect the bcc-Mo+T2 (Mo_5SiB_2)-based alloys to develop potentially oxidation resistant alloys. Two different coating processes were investigated. First, the T1-based alloy was plasma-sprayed onto Mo substrates to determine the feasibility of protecting the bcc-Mo+T2(Mo_5SiB_2)-based alloys. This work showed that air plasma spraying leads to excessive loss of Si, shifting the overall phase assemblage of the coating to a T1+T2 composition. The microstructural evolution of the coating upon annealing was studied. The second coating strategy involved siliconizing the surface of the bcc Mo-based alloy by the halide activated pack-cementation (HAPC) process. This vapor-phase process deposits Si onto the surface of the alloy, which reacts at the deposition temperature of 900˚C to form a conformal layer of $MoSi_2$. The microstructure and oxidation resistance of the coating were investigated as a function of HAPC processing parameters.

Keywords: Coatings, Alloys, Oxidation

290. MICROSTRUCTURAL EVOLUTION OF TIAL-INTERMETALLIC ALLOYS CONTAINING W AND B (UT-2A)
$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 Tennessee Contact: P. K. Liaw, 865-974-6356

The TiAl alloys have been considered as promising candidates for structural applications at around 800^{0}C. In this work, new TiAl alloys, containing tungsten (W) and boron (B), have been developed. Using the scanning-electron microscopy (SEM), electron-microprobe, and transmission-electron microscopy (TEM), the effects of W and B on the microstructural evolution of TiAl alloys, including colony size and lamellar spacing, were analyzed. It is important to point out that fine, uniform microstructures (with a colony size smaller than 50 mm) can be conveniently developed after hot-isostatic pressing (HIP) of the as-cast alloys at 1,250^{0}C and 150 MPa for 4 h without the deformation process. It was found that tungsten prefers to react with boron to form borides, and disperses mainly along grain boundaries, and occasionally inside grains. With an increase of the tungsten content, the microstructure can be further refined. Heat treatments at temperatures ranging from 900^{0}C to 1,310^{0}C were conducted. The addition of tungsten can restrain the grain coarsening, and stabilize the microstructure up to 1,280^{0}C by hindering the migration of grain boundaries at high temperatures. It is also noteworthy that the beta phase, a high-temperature ductile phase, forms when the tungsten content exceeds 0.4 atomic percent (at.%). The α-phase transus temperature, T_α, has been determined through differential-thermal analysis (DTA) and further proved by investigation of the microstructural changes during various heat treatments. Different microstructures meeting desirable needs can be developed through heat treatments beyond and below the α-phase transus temperature. Mechanical testing, such as hardness measurement, has been conducted on the alloys. The addition of tungsten increases the hardness of TiAl alloys by solution strengthening and refinement of grain size.

Keywords: Intermetallics, Alloys, Microstructure

291. NOVEL STRUCTURES AND PROPERTIES THROUGH CONTROLLED OXIDATION (ORNL-4A)
$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: M. P. Brady, 865-574-5153

The goal of this program is to explore novel routes for controlling the chemistry and architecture of near-surface oxidation (nitridation, carburization, etc.) products that have application in advanced fossil-fuel fed systems by manipulating precursor alloy composition and microstructure. The effort will focus on gaining an understanding of the conditions under which the oxidation of multi-component, single-phase and multi-phase alloys can (1) controllably yield complex (ternary and higher order) ceramic phases in layered or dispersed (composite) arrangements of interest for functional applications (e.g. catalysts, gas sensors, etc.) and (2) establish continuous simple (binary-scales for protection in aggressive, high-temperature environments, i.e. selective oxidation. The proposed program will primarily be based on studies of model systems selected from phenomenological as well as scientific considerations. However, a major aim of the program is to serve as an incubator for the spin-off of new processes and materials into targeted development efforts relevant to, and needed for, the building blocks of future efficient, economic fossil fuel power plants with substantially reduced emissions. The alloy development aspects of the efforts to form protective surface layers are linked from a technical standpoint with WBS element 2D, Multi-phase high-temperature alloys.

292. CONCEPTS FOR SMART, PROTECTIVE, HIGH-TEMPERATURE COATINGS (ORNL-4C)
$120,000
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

Environmental resistance is a critical material barrier to the operation of fossil-fuel systems with breakthrough energy utilization and environmental performance being sought by the Office of Fossil Energy. All fossil fuel-derived processes contain reactive species (often more than one), and high-temperature degradation arising from multiple reactions of solids with gases and condensable products often limits performance or materials lifetimes such that efficiency, emission, and/or economic targets or requirements are not realized. This project is somewhat different from traditional corrosion-resistant coating studies in that it focuses on the feasibility of routes to controlling the critical chemical and mechanical phenomena that collectively form the basis for environmental protection in relevant fossil environments. It does this by exploring compositional and microstructural manipulations and cooperative phenomena that have not necessarily been examined in any detail to date. This can hopefully lead to concepts for "smart" coatings or materials that have the ability to sense and respond appropriately to a particular set or series of conditions in order to provide high-temperature corrosion protection in multiple-reactant and/or varying high-temperature environments.

The first concepts being explored involved bulk, multiphase molybdenum silicides, which showed low corrosion rates under sulfidizing conditions simulating an aggressive coal syngas (H_2-H_2S-H_2O-Ar) environment. The results were consistent with expected behavior of the Mo-Si system based on thermodynamic and kinetic factors. Similar considerations were used in evaluating multiphase Ti-Al-Cr-X compositions, where X = Ta, Nb, or C, with a focus on understanding how the compositional and microstructural characteristics of these alloys can be manipulated to assure that surface products stable and protective in the syngas environment form. Initial results from 800˚C exposures of Ti-Al-X compositions to dry air and the sulfidizing environment have been obtained, with preliminary analyses showing generally good oxidation and sulfidation resistance.

Keywords: Coatings, High Temperature

293. DEVELOPMENT OF A COMMERCIAL PROCESS FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS (REMAXCO-5)
$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
ReMaxCo Technologies, Inc. Contact:
R. D. Nixdorf, 865-483-5060

Single crystal silicon carbide fibrils have exhibited oxidation resistance to 1,600ºC and 5X mechanical properties performance over other commercial silicon carbide fibers. The high-temperature properties of the fibrils will provide an advantage to the Department of Energy's Fossil Energy Program in the areas of heat exchanger tubes, recuperative components and hot gas filters in advanced, coal-fired combustion plants. A manufacturing process for these fibrils with the potential for low-cost and high-volume fibril production is being investigated. The initial phase of this development program in FY 2000 demonstrated the feasibility of microwave-assisted fibril synthesis on a bench-scale. The second phase in FY 2002 focused on the operation of a pilot-scale, semi-continuous fibril growth furnace, which exhibited significant problems in microwave-heating uniformity and reactant gas feed control. The current FY 2004/2005 development phase reaction vessel is designed to eliminate those deficiencies. Expert companies in microwave field control and CVD gas feed systems have been contracted to design and build the new reactor. The new reactor fabrication has been completed. It is currently in the debugging process and will be in a start-up mode by June 2005. A New York company skilled in the use of SiC precursor materials and CVD processing has agreed to install the reactor in their facility for potential future fibril volume production in a joint venture with ReMaxCo. Significant interest in the fibrils product, beyond the fossil energy applications, is being expressed in the areas of machine cutting tools, high-performance computer chip carriers, and military vehicle lightweight composites.

Keywords: SiC, Fibrils, Composites

294. ADVANCED PROCESSING OF METALLIC POWDERS (AMES-3)
$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: I. Anderson,
515-294-4446

This project seeks to enhance the control of metal powder production by gas atomization methods, to benefit the implementation of several emerging Fossil Energy technologies that utilize metal powders of specific size ranges and types, but which are not efficiently produced by industrial powder makers. Further improvements in fundamental understanding and design of high-efficiency gas atomization nozzles is directed toward maximizing powder yields in special size classes, including ultra fine (dia. <10 µm) and mid-range (10-75 µm) powders, with reduced standard deviation. Efficient production of such powders can eliminate a major technological barrier to the use of new concepts for fabrication of hydrogen membranes or thermal sprayed coatings of oxidation resistant alloys, for example. To provide a direct route for rapid transfer of the atomization technology improvements, powder production tests were performed in an up-scaled industrial prototype atomization system. Starting with the atomization gas supply system, the industrial prototype atomization system will be fully adapted to a level consistent with advanced, industrial operation in terms of steady-state operation and control systems. These adaptations are needed to permit increased powder batch sizes, and to remove ambiguity in the detection of nozzle performance response to parameter modifications, making every experiment more useful for verification of design concepts. Benchmark trials on some Fe-based alloys, including Fe-16Al-2Cr (wt.%) and Fe-12Cr-1Y (intended for Fossil Energy applications) were performed initially to provide assurance that significant improvements can be achieved. In addition, some results will be reported on parallel work involving controlled sintering (into thin porous sheets) of ultra-fine spherical alloy powders, exploring their application as support structures for various types of hydrogen membranes.

Keywords: Powder Metallurgy, Alloys, Fe-Base

ADVANCED METALLURGICAL PROCESSES PROGRAM

The materials program at the Albany Research Center (ARC) incorporates Advanced Metallurgical Processes that provide essential life-cycle information for evaluation and development of materials. The research at ARC directly contributes to FE objectives by providing information on the performance characteristics of materials being specified for the current generation of power systems, on the development of cost-effective materials for inclusion in the next generation of fossil fired power systems, and for solving environmental emission problems related to fossil fired energy systems. The program at ARC stresses full participation with industry through partnerships and emphasizes cost sharing to the fullest extent possible.

The materials research in the Program focuses on extending component service lifetimes through the improvement and protection of current materials, by the design of new materials, and by defining the service operating conditions for new materials in order to ensure their safe and effective use. This process involves developing a better understanding of specific failure modes for materials in severe operating environments, addressing factors which limit their current use in these environments, and by designing new materials and materials processing procedures to overcome anticipated usage challenges in severe operating environments, such as those typically found in fossil energy generating plants and in structures and supporting facilities associated with oil and gas production. Emphasis is placed on high-temperature erosion testing and modeling in environments anticipated for FutureGen programs, development of casting technologies and new alloys to improve wear resistance in those environments, and on repair and development of refractory materials for coal gasifiers. DOE contact is Alan D. Hartman, 541-967-5862.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

295. ADVANCED FOIL LAMINATION TECHNOLOGY
$600,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact:
Arthur V. Petty, Jr., 541-967-5878

ARC researchers have developed a materials fabrication approach that utilizes dissimilar foils to produce a variety of materials (e.g., layered composites, monolithic metallic and intermetallic alloys). The research has identified bonding parameters for laminating type 347-stainless steel foils. This technique has also been used to join dissimilar metals. The goal of this research is to use conventional deformation processing techniques (such as extrusion or rolling) to bond foils to substrates and to each other. (This research was completed in FY 2004.)

Keywords: Aluminides, Coatings, Foil-Lamination Process

296. ADVANCED CASTING TECHNOLOGIES
$400,000
DOE Contact: Alan D. Hartman, 541-967-5862
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, Refractory Metals

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

297. ADVANCED REFRACTORIES FOR SLAGGING GASIFIERS
$600,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact: Cindy A. Powell, 541-967-5803

The emphasis of this high temperature material research has been driven by both short-range industrial needs and long-range issues in gasifiers. Program emphasis is on: 1) identifying material failure mechanisms, 2) identifying/developing materials that will extend the lifetime of primary refractory liners in slagging gasifier systems, 3) developing repair techniques to shorten system downtime caused by refractory maintenance, and 4) developing improved thermocouples/temperature-monitoring techniques. A refractory material with improved resistance to attack by molten coal slags in simulated gasifier environments has been developed.

Keywords: Refractories, Slagging Gasifier, Liners, Thermocouples

298. LOW-CHROME/CHROME FREE REFRACTORIES FOR SLAGGING GASIFIERS
$400,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contacts:
Cindy A. Powell, 541-967-5803

The focus of this research will be to develop low-chrome oxide and/or no-chrome oxide refractory liner materials for slagging gasifiers. The driving forces for this research are: 1) high Cr_2O_3 containing refractories have not met the service life requirements of gasifier users, 2) the high cost of refractory materials that contain large percentages of Cr_2O_3, and 3) the possible long-term supply issues associated with refractory producers who currently manufacture chrome based refractory materials but may choose to cease production because of the impact of future EPA and OSHA regulations on the production, use, or disposal of chrome containing materials. Project research investigates the role chrome oxide plays in gasifier refractories, evaluates wear mechanisms and non-chrome or low-chrome high temperature refractory oxides with potential use in combating those wear mechanisms in gasifier refractories. The project intends to conduct field tests of engineered refractory materials.

Keywords: Refractories, Chromium, Chrome Oxides

299. STEAM TURBINE MATERIALS AND CORROSION
$300,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact: Cindy A. Powell, 541-967-5803

As progress is made in fossil energy power production in terms of overall efficiency, issues arise as to the ability of existing structural materials to withstand the higher operating temperatures and pressures in advanced power plants. This project is focused on the development of high strength austenitic or superalloys for use in ultra supercritical steam turbines. Steam-side corrosion tests will be conducted on candidate materials. Emphasis will also be placed on determining the effect of pressure on the corrosion process. Temperatures and pressures of up to 1400˚F (760˚C) and 5000 psi (34.5 MPa) will be subjected to candidate materials to determine performance.

Keywords: Corrosion, Steam, Superalloys, Turbines, High Temperature, High Pressure

300. ABRASION AND EROSION OF MATERIALS FOR FOSSIL ENERGY SYSTEMS
$250,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact: Cindy A. Powell, 541-967-5803

Abrasion and erosion are significant materials-related problems found in the operation of fossil energy plants. By understanding the general wear, abrasion, 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

301. SENSORS TO DETECT CORROSION UNDER ASH DEPOSITS
$1,000,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact: Cindy A. Powell, 541-967-5803

Research will be conducted to develop novel high temperature electrochemical corrosion rate sensors and to determine the accuracy of their measured corrosion rates and the stability of the sensors over extended periods of use. Research in support of this will focus on the interactions between the gas phase, ash, and metal surfaces in typical combustion (coal and waste) and gasification environments. The goal of the research will be to transfer electrochemical corrosion rate sensor technology to the power generation industry along with a thorough understanding of the limitations and uses of these sensors.

Keywords: Corrosion, Molten Salts, Hot Corrosion, Sensors

302. METALLIC MATERIALS DEVELOPMENT FOR SOLID OXIDE FUEL CELL APPLICATIONS
$1,100,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact: Paul C. Turner, 541-967-5863

The ultimate goal of the materials development program is to develop nickel-base alloys with low thermal expansion (low CTE) to transition from solid oxide fuel cells to balance of plant heat exchangers and ancillary equipment. These nickel-base alloys developed will be investigated for suitability within solid oxide fuel cell applications.

Keywords: Oxidation, Corrosion, Fuel Cell, Alloys

303. MATERIALS PERFORMANCE FOR HEAT EXCHANGERS & OTHER BALANCE OF PLANT COMPONENTS FOR SOLID OXIDE FUEL CELLS
$900,000
DOE Contact: Alan D. Hartman, 541-967-5862
Albany Research Center Contact: Paul C. Turner, 541-967-5863

The chief characteristic of fuel cells is the ability to convert chemical energy to electrical energy without the need for combustion, giving much higher conversion efficiencies than conventional methods. Costs of fuel cells remain an issue and can be reduced in component fabrication, materials used, and cell and stack designs. However, balance of plant issues also present problems in the commercialization of fuel cell technology. Specifically for solid oxide fuel cells, air and fuel need to be heated and cooled at some stage of the process. This requires pumps, piping, heat exchangers, etc. in order to deliver useable electrical power. Currently, there are no economical commercial heat exchangers suitable for use with solid oxide fuel cells. This project will explore materials of construction and heat exchanger designs as a means of developing a low cost high temperature heat exchanger for solid oxide fuel cell systems.

Keywords: Oxidation, Corrosion, Fuel Cells, Heat Exchangers

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
SC-32/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-2917

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-35/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-8379

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

Kristin Bennett
SC-12/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-4269

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

Robert Boettner
EM-3.2/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-7437

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

Altaf Carim
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-4895

R. W. Carling, Div. 8313
Sandia National Laboratories
Livermore, CA 94550
(925) 422-2206

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
NA-233/GTN
U.S. Dept. of Energy
Washington, DC 20545
(301) 903-1456

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

John Cooke
Solid State Division
Oak Ridge National Laboratory
PO Box 2008
Oak Ridge, TN 37831
(865) 574-5787

Alastair N. Cormack
NYS College of Ceramics
Alfred University
Alfred, NY 14802
(607) 871-2180

George Crabtree
Material Science Division
Argonne National Laboratory
9700 South Cass Aveneue
Argonne, IL 60439-4841
(630) 252-5509

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

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
FE-22/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-2700

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) 252-5032

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-2D/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-9154

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-21/FORS
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-7282

Ehr-Ping Huang Fu
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
P.O. Box 1663/MST
Los Alamos, NM 87545
(505) 664-0980

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) 275-4455

S. H. Goods
Divison 8314
Sandia National Laboratories
Livermore, CA 94550
(925) 422-3274

R. J. Gottschall
SC-13/GTN
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-3978

Anton C. Greenwald
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

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

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

Bruce Harmon
Ames Laboratory
Ames, IA 50011
(515) 294-5772

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

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

James Horwitz
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-4894

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

Robert Hwang
Brookhaven National Laboratory
Upton, NY 11973
(631) 344-3322

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
NA-115.2
U.S. Dept. of Energy
Washington, DC 20585
(301) 903-4236

Landis Kannberg
Pacific Northwest Natl Lab
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

Richard Kelley
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-6051

Helen Kerch
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-2346

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

Aravinda Kini
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-3565

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

Harriet Kung
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-1330

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 (NETL-PGH)
P.O. Box 10940
Pittsburgh, PA 15236
(412) 386-4664

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

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
(925) 423-7051

Patrick N. McDonnell
Spire Corporation
One Patriots Park
Bedford, MA 01730-2396
(617) 275-6000

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

Pedro Montano
SC-12/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-2347

Andrew Morrison
M/S 238-343
Flat Plate Solar Array Project
Jet Propulsion Laboratory
Pasadena, CA 91109
(213) 354-7200

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) 275-3050

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

William Oosterhuis
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-4173

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

Don Parkin
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-9243

Bill Parks
TD-1/FORS
U.S. Dept. of Energy
Washington, DC 20585
(202) 586-6623

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) 275-4441

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

George Samara
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-6653

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 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

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-24/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

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
EA-1/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

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
SC-20/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

Lou Terminello
L-353
LLNL
PO Box 808
Livermore, CA 94551
(925) 423-7956

Pat Thiel
Ames Laboratory
Iowa State University
Ames, IA 50011
(515) 294-8985

Bruce Thompson
Ames Laboratory
Iowa State University
Ames, IA 50011
(515) 294-7864

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
(630) 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
Washington, DC 20585
(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

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

David Welch
Brookhaven Natl Lab
PO Box 5000
Upton, NY 11973-5000
(631) 344-3517

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

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

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 20585
(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
National Energy Tech Lab (NETL-MGN)
Gas Supply Projects Division
3610 Collins Ferry Road
Morgantown, WV 26507-0880
(304) 285-4265

Jane Zhu
SC-13/GTN
U.S. Department of Energy
Washington, D.C. 20585
(301) 903-3811

Kenneth Zwiebel
NREL
1617 Cole Blvd
Golden, CO 80401
(303) 384-6441

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