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ENERGY MATERIALS COORDINATING COMMITTEE (EMaCC)

Fiscal Year 2005

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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 5-7.

Seven meetings were scheduled for 2005-2006. The dates and minutes from the meetings are as follows:

MEETING MINUTES OF MAY 4, 2005

The EMaCC meeting was held in room G-426 in the Germantown Building. The meeting started at 10:15 A.M. and ended at 11:30 A.M. The Chairwoman, Dr. Jane Zhu, opened the meeting with the participants introducing themselves.

Carole J. Read (EE-2H) talked about the DOE Hydrogen Program: EERE Research Plans and Projects for Hydrogen Storage. The current state of the art in hydrogen storage was presented as well as 5 and 10 year performance goals which have been set for the program. An overview of the organization of the National Hydrogen Storage project and the enters of Excellence were presented. Jim Horwitz (SC/BES) talked about the recent BES Workshop on Basic Research Needs for Effective Solar Energy Utilization. Over 200 participated in the successful meeting and the final report will be issued in August 2005. Some of the conclusions of the workshop were: significant research and development is required to develop renewable solar technologies; the research is highly interdisciplinary; and basic and applied research needs to be strongly coupled. The minutes of the meeting held on February 8, 2005 were approved.

CALENDAR ITEMS

September 13-15: Merit Review of the Heavy Vehicle Materials Program at the Oak Ridge National Laboratory in Oak Ridge, TN. http://www.eere.energy.gov/vehiclesandfuels/resources/fcvt_hswr_fy04.shtml

MEETING MINUTES OF JUNE 28, 2005

The EMaCC meeting was held in room E-401 in the Germantown Building. The meeting was started at 10:10 A.M. and ended at 11:40 A.M. The special topic of this meeting was *Superconductivity*. The Chairwoman, Dr. Jane Zhu, opened the meeting with the participants introducing themselves.

Jim Daley (OE-10) gave an overview of the superconductivity program for electric power applications. The mission of the program is to work in partnership with industry to develop high temperature superconducting (HTS) wire and perform pre-commercial R&D activities required for U.S. companies to commercialize HTS electric power applications. An overview of the current state of the art was presented, as well as the need for dielectric materials and cryogenic equipment research. Bill Oosterhuis (SC-22.2) talked about basic research activities in superconductivity. These activities include materials discovery, characterization, and the use of modeling and experimentation to understand mechanisms. Bruce Strauss (SC-25.1) talked about superconductivity applications in high energy physics and presented the history of the development of superconductors. Jim Horwitz (SC-22.2) led a discussion on the upcoming superconductivity workshop. Input from the committee was given regarding workshop goals, candidates for chair, panel topics and potential chairs, and possible workshop dates.

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MEETING MINUTES OF SEPTEMBER 7, 2005

The EMaCC meeting was held in room GH-027 in the Forrestal Building. The meeting was started at 10:15 A.M. and ended at 12:00 P.M. The Chairwoman, Dr. Jane Zhu, opened the meeting with the participants introducing themselves.

Dave Howell presented for Tien Duong (EERE) on materials research in for lithium batteries. The current state of the art was discussed as well as the performance goals that are planned to be achieved by 2010. The main issues with these technologies are cost, lifetime, and ability to perform/charge in various environments. Matesh Varma (SC/BES) presented an overview of the Department Experimental Program to Stimulate Competitive Research (EPSCoR). His discussion included a history of the program and how program offices, laboratories, and universities all benefit from participation. For more information: www.sc.doe.gov/bes/EPSCoR/index.htm. The minutes of the EMaCC meetings held on May 4 and June 28 were approved with amendments.

CALENDAR ITEMS

ASM International Conference: September 25-29, 2005, Pittsburgh, Pennsylvania.

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MEETING MINUTES OF OCTOBER 12, 2005

Energy Materials Coordinating Committee (EMaCC) Special Topic Meeting on *Materials for Pushing Performance Envelopes under Extremes of Temperature, Corrosion, Irradiation and Applied Stress*

The meeting was held in room E-301 in the Germantown Building. The meeting was started at 10:15 A.M. and ended at 12:30 P.M. The Chairwoman, Dr. Jane Zhu, opened the meeting with the participants introducing themselves.

Bob Gottschall (SC/BES) discussed research to understand the lack of ductility in intermetallics, corrosion studies, and plutonium immobilization. Sue Lesica (NE) gave an overview of materials research in NE, including materials for the next generation of nuclear reactors. Bob Finch (ANL/RW) presented research on amorphous coatings for possible use on the drip shields in a geologic repository. Gene Nardella (SC/FES) presented an overview of the ITER project and the materials research being performed to support the U.S. contribution to the international project. Udaya Rao (FE) discussed the FutureGen program and research into high temperature structural materials for the production of hydrogen from coal.

CALENDAR ITEMS

Next EMaCC meeting December 13, 2005.

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MEETING MINUTES OF DECEMBER 13, 2005

The EMaCC meeting was held in room E-114 in the Germantown Building. The meeting started at 10:15 A.M. and ended at around 12:00 P.M. The Chairperson, Dr. Jane Zhu, opened the meeting with the participants introducing themselves.

John Fairbanks (EE-2G) made a presentation on the thermoelectric research program within the DOE FreedomCAR & Vehicle Technologies Program. He described opportunities for high efficiency thermoelectrics R&D in fuel savings applications. Thermoelectric materials are needed in vehicle technologies that can recover and convert engine waste heat to electrical energy to improve overall engine efficiency. Both an overview of the program and technical highlights were presented. Prof. Terry Tritt (Clemson University) presented a talk on the thermoelectrics research being conducted under his leadership in a statewide (South Carolina) project funded by DOE-EPSCoR. He presented an overview of the thermoelectric phenomenon, applications, and new directions in bulk thermoelectric materials research. New officers for 2006 were elected: Sue Lesica (NE-20) as the Chairperson and Aravinda Kini (SC-22.2) as Executive Secretary. The minutes of the meeting held on September 7, 2005 were approved. Hydrogen embrittlement was suggested as a topic of discussion for a future meeting.

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MEETING MINUTES OF MARCH 22, 2006

The EMaCC meeting was held in room GH-027 in the Forrestal Building. The meeting started at 10:15 A.M. and ended at around 12:00 P.M. The Chairperson, Dr. Sue Lesica, opened the meeting with the participants introducing themselves. Prof. Ian Robertson, Head, Department of Materials Science and Engineering, University of Illinois-Urbana Champaign made a presentation entitled Hydrogen Embrittlement From Fundamental Understanding to Engineering Practice He described both the historical aspects of and recent advances in understanding the mechanics of hydrogen embrittlement, which often involve multiple failure mechanisms in the *same* material. This knowledge is critically needed in the design of containers for hydrogen storage, an area of high current interest for the DOE. Next, Dr. James Brodrick, Manager of the Solid State Lighting Program in the Office of Building Technologies, EERE, presented an overview of the Solid State Lighting Portfolio and Materials Development. The minutes of the meeting held on December 13, 2005, were approved.

Several calendar items of potential interest were brought up. Carol Reed-Hydrogen program meeting/review on May 16-19, 2006; Aravinda Kini-BES Workshop on Basic Research Needs in Solid State Lighting on May 22-24, 2006.

Potential speakers and topics for the next meeting were suggested. Dick Kelley suggested George Crabtree to provide an update on the Lab Working Group activities; Sara Dillich suggested Bob O'Connell to speak on the materials issues/needs in solar energy conversion.

The meeting adjourned at 12:00 P.M.

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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 2005 and describes the materials research programs of various offices and divisions within the Department.

The EMaCC Chair for FY 2005 was Dr. Jane Zhu. The compilation of this report was performed by Dr. Aravinda Kini, EMaCC Executive Secretary for FY 2006, 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. Susan Lesica
Office of Nuclear Energy
EMaCC Chair, FY 2006

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
	Richard Kelly, SC-22.2	301-903-6051
Condensed Matter Physics and Materials Chemistry	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, SE-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
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	Bob Lange, NE-40	301-903-2915
Space and Defense Power Systems	John Dowicki, NE-50	301-903-7729

ORGANIZATION	REPRESENTATIVE	PHONE NO.
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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 2005 budget summary for DOE Materials Activities is presented on page 9. The distribution of these funds between DOE laboratories, private industry, academia and other organizations is presented in tabular form on page 11.

Following the budget summary is a set of detailed program descriptions for the FY 2006 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 2005 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 2005 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 2005
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS	$8,517,000
FREEDOMCAR & VEHICLE TECHNOLOGIES PROGRAM	$36,477,000
Transportation Materials Program	35,902,000
Automotive Propulsion Materials	1,775,000
Automotive Lightweight Materials (ALM)	16,260,000
Heavy Vehicle Propulsion Materials	4,075,000
High Strength Weight Reduction (HSWR) Materials	7,692,000
High Temperature Materials Laboratory	6,100,000
Electric Vehicle R&D Program	575,000
Advanced Battery Development	575,000
GEOTHERMAL TECHNOLOGIES PROGRAM	$335,000
Geothermal Materials	335,000
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM	$20,368,055
Fuel Cell Materials	625,000
Hydrogen Production Materials Program	1,950,000
Hydrogen Storage Materials Program	17,793,055
INDUSTRIAL TECHNOLOGIES PROGRAM	$11,264,946
Aluminum Subprogram	1,940,478
Metal Casting Subprogram	819,468
Steel Subprogram	NA[1]
Materials Subprogram	8,505,000
SOLAR ENERGY TECHNOLOGY PROGRAM	$28,638,000[2]
Office of Solar Energy Technologies	28,638,000
National Photovoltaics Program	28,638,000
OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION	$36,000,000
High Temperature Superconductivity for Electric Systems	36,000,000

[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 FY05 funding data are not available.

[2]This is the total materials research component of the National Photovoltaics Program.

FY 2005 BUDGET SUMMARY OF DOE MATERIALS ACTIVITIES (continued)

	FY 2005
OFFICE OF SCIENCE	$741,868,297
Office of Basic Energy Sciences	686,700,000
Division of Materials Sciences and Engineering	247,914,000
Division of Scientific User Facilities	438,786,000
Office of Advanced Scientific Computer Research	45,369,297
Technology Research Division	45,369,297
Small Business Innovation Research Program	42,948,439
Small Business Technology Transfer Research Program	2,420,858
Office of Fusion Energy Sciences	8,600,000
Office of Biological & Environmental Research	1,199,000
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY	$11,272,340
Office of Space and Defense Power Systems	6,827,340
Space and National Security Programs	6,827,340
Office of Advanced Nuclear Research	4,445,000
Advanced Fuel Cycle Initiative	1,815,000
Nuclear Hydrogen Initiative	2,630,000
NATIONAL NUCLEAR SECURITY ADMINISTRATION	$118,126,000
Office of Naval Reactors	66,600,000[1]
Office of Defense Programs	51,526,000
The Weapons Research, Development and Test Program	51,526,000
Sandia National Laboratories	34,066,000
Lawrence Livermore National Laboratory	8,100,000
Los Alamos National Laboratory	9,360,000
OFFICE OF FOSSIL ENERGY	$12,543,000
Office of Advanced Research	12,543,000
Advanced Research Materials Program	6,978,000
Advanced Metallurgical Processes Program	5,565,000
TOTAL	$1,025,409,638

[1]This excludes $67.5 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

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

TABLE 2
DISTRIBUTION OF FUNDS BY OFFICE

Office	DOE Laboratories	Private Industry	Academia	Other	Total
Office of Building Technology, State and Community Programs	$5,491,000	$720,000	$2,306,000	$0	$8,517,000
FreedomCAR & Vehicle Technologies Program	$22,597,000	$9,888,000	$2,277,000	$1,715,000	$36,477,000
Geothermal Technologies Program	$335,000	$0	$0	$0	$335,000
Hydrogen, Fuel Cells and Infrastructure Technologies Program	$8,793,000	$5,331,055	$5,439,000	$805,000	$20,368,055
Industrial Technologies Program	$7,250,549	$2,046,150	$1,968,247	$0	$11,264,946
Solar Energy Technology Program	$28,638,000	$0	$0	$0	$28,638,000
Office of Electric Transmission and Distribution	$18,700,000	$16,000,000	$1,280,000	$20,000	$36,000,000
Office of Science	$474,689,000	$45,369,297	$221,810,000	$0	$741,868,297
Office of Nuclear Energy, Science and Technology	$8,642,340	$0	$2,630,000	$0	$11,272,340
National Nuclear Security Administration	$118,126,000	$0	$0	$0	$118,126,000
Office of Fossil Energy	$10,961,000	$192,000	$765,000	$625,000	$12,543,000
TOTALS	**$704,222,889**	**$79,546,502**	**$238,475,247**	**$3,165,000**	**$1,025,409,638**

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.

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

	FY 2005
OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS TOTAL	$8,517,000
SOLID STATE LIGHTING	6,724,000
Novel Materials for High-efficiency White Phosphorescent Organic Light Emitting Diodes	1,350,000
Development of White-light Emitting Active Layers in Nitride-based Heterostructures for Phosphorless Solid State Lighting	956,000
Novel Organic Molecules for High-efficiency Blue Organic Electroluminescence	2,400,000
Material and Device Designs for Practical Organic Lighting	2,018,000
FENESTRATION MATERIALS DEVELOPMENT	$1,220,000
Development of “Electrochromic” Materials and Coatings	1,220,000
NEW BUILDING MATERIAL DEVELOPMENT AND HYGROTHERMAL MODELING	$573,000
Phase Change Material (PCM)-Enhanced Cellulose Based Insulation	150,000
Hygrothermal Property Measurements & Modeling Upgrades and Applications	423,000

OFFICE OF BUILDING TECHNOLOGY, STATE AND COMMUNITY PROGRAMS

PROGRAM GOALS

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

PROGRAM OBJECTIVES

The program objectives are:

- Develop a new generation of solid state lighting sources that can double today's most efficient products
- Develop Advanced Windows that have highly insulating properties, that offer dynamic solar heat gain control, and have very low solar heat gain coefficients
- Identify and develop new or improved insulation and other building materials
- Develop and standardize laboratory methods for characterizing new and existing materials
- Develop a fundamental understanding of the physics of heat, air, and moisture flow in advanced and conventional building materials

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

SOLID STATE LIGHTING

1. NOVEL MATERIALS FOR HIGH-EFFICIENCY WHITE PHOSPHORESCENT ORGANIC LIGHT EMITTING DIODES
   $1,350,000
   DOE Contact: Dr. James Brodrick, (202)-586-1856
   University of Southern California Contact:
   Dr. Mark Thompson, (213) 740-6402

This project involves a materials synthesis effort, in which large families of materials will be generated, intended for use in each of the different parts of the OLED. Each of the materials will be prepared with a specific device concept in mind, which involves resonant injection of carriers into the emissive layer. The materials to be prepared and examined here include carrier transporting/injecting materials, host materials for the doped emissive layer, and phosphorescent dopants, in a range of colors as well as broadband emitters. All of these materials will be extensively screened for chemical and thermal stability before being incorporated into OLEDs. OLED testing will be done in both monochromatic and white OLED structures. Many of the materials being prepared in this program will be useful in a range of different OLED structures and could be adopted by other research groups and programs to enhance the efficiency and stability of their devices.

The device architecture used in this program will rely on several specific design criteria to achieve high efficiency and long lifetime. The use of phosphorescent dopants will be necessary in any OLED structure to meet the DOE's performance goals. The emissive materials are all phosphorescent complexes, which have demonstrated long device lifetimes and high efficiencies in monochromatic devices, which are expected to carry over to properly designed white devices. The weak link in these materials is the blue phosphorescent dopant. These materials will be specifically targeted, and have a sound strategy to solve the blue reliability problems. In addition to designing the optimal monochromatic and broadband phosphors for the devices, a controlled energetic alignment for the devices will be relied upon, which will minimize drive voltage and increase the exciton formation efficiency. The carrier-injecting materials will be chosen to match the HOMO and LUMO levels in the emissive dopant exactly, such that the carriers are injected into the phosphorescent dopant in a resonant process. The phosphor will be doped into a wide gap host material, which will prevent host-carrier interactions, keeping the carriers and excitons exclusively localized on the phosphors.

Keywords: Solid State Lighting, Light-Emitting Diodes, Organic Light-Emitting Diodes, Phosphors

2. DEVELOPMENT OF WHITE-LIGHT EMITTING ACTIVE LAYERS IN NITRIDE-BASED HETEROSTRUCTURES FOR PHOSPHORLESS SOLID STATE LIGHTING
   $956,000
   DOE Contact: Dr. James Brodrick, (202)-586-1856
   University of California, San Diego Contact:
   Jan Talbot

Building upon earlier work supported by DOE at the University of California at San Diego, researchers are using novel, combustion-produced activators to stimulate photonic emissions for otherwise non-radiative relaxation pathways. Early demonstrations of this important concept will be done on thin films using a laser ablation technique, but the potential to use the approach in the design of a practical LED heterostructure will also be explored. This work could have a dramatic impact on traditional nitride devices by substantially improving internal quantum efficiencies by as much as 30%, with virtually no added manufacturing complexity or cost.

This new effort is a collaboration between UC San Diego (PI: Prof. J. McKittrick) and OSRAM SYLVANIA (Dr. K. Mishra). The main objective is to develop a new LED architecture using thin films of nitride-based luminescent semiconductor alloys of GaN, AlN, and InN, and suitably chosen activator ions to produce white light. The activator ions will consist of one or two types of ions that, together and with band edge emission from the alloy, will yield a superposition of emission spectra from the individual activator ions and lead to a white-light emitter with high efficacy and color rendering index. These activator ions are presumed to be excited by energy transfer from the electron-hole (e-h) pairs generated in the semiconducting dies. Such a thin film can be used as an active layer in designing double heterojunctions for solid-state lighting applications. Research activities are planned to demonstrate that such an alloy can be designed by adjusting the alloy composition and activator ions, that nonradiative energy transfer from the e-h pairs to the activator ions would occur efficiently (Phase I), that thin films of such an alloy would retain the efficacy in powder form (Phase II), and that a chemical reaction route can be found to grow a thin film of this alloy epitaxially on a p- or n-type material (Phase III). The last step is critical for integrating this technology, when successfully developed, to the existing manufacturing processes of nitride-based LED systems.

Keywords: Solid State Lighting, Light-Emitting Diodes, Heterostructures

3. NOVEL ORGANIC MOLECULES FOR HIGH-EFFICIENCY BLUE ORGANIC ELECTROLUMINESCENCE
   $2,400,000
   DOE Contact: Dr. James Brodrick, (202)-586-1856
   Pacific Northwest National Laboratory Contact:
   Paul Burrows, (509) 375-5990

This project explores using-state-of-the-art phosphorescent organic light emitters to dramatically increase the power efficiency of blue organic light emitting devices by incorporating them in novel, electron-transporting host layers. Blue is thought by many to be the color that limits the efficacy of white OLED devices, as well as full-color organic light emitting displays. Typically, organic phosphors are doped into a conductive host matrix and emission results from energy transfer from the host to the triplet state of the phosphor. Development of efficient blue OLEDs based on this technology has been particularly challenging because the host material must exhibit triplet level emission of 450 nm without sacrificing charge transporting properties. Current host materials do not meet these requirements because there is a tradeoff between increasing the bandgap of the material and decreasing the p-aromatic system, which adversely affects charge transport properties. Deeper blue phosphors have only been demonstrated in insulating, wide bandgap host materials with charge transport occurring via hopping between adjacent dopant molecules. This leads to high voltage and, therefore, less efficient devices.

An alternative route for achieving blue shifted emission energies is to replace the nitrogen heteroatoms with phosphorus. For example, aromatic diphosphine oxides are stable compounds that exhibit electroluminescence in the ultraviolet spectral region (335 nm for one example already tested) while extended electronic states in the phosphorus atom give rise to good electron transport at low voltages. Thus, it is possible to widen the bandgap without eliminating the aromatic backbone of the molecule, which makes these materials excellent hosts for high-efficiency blue phosphors, as well as longer wavelength OLEDs.

Keywords: Solid State Lighting, Light-Emitting Diodes, Organic Light-Emitting Diodes, Phosphors

4. MATERIAL AND DEVICE DESIGNS FOR PRACTICAL ORGANIC LIGHTING
   $2,018,000
   DOE Contact: Dr. James Brodrick, (202)-586-1856
   Los Alamos National Laboratory Contact:
   Darryl Smith, (505) 667-2056

This project will combine theoretical and experimental approaches to methodically address key material challenges for OLED use in general illumination applications. The project will systematically advance the physical and chemical understanding of how materials-related phenomena can be altered to make very high efficiency, low voltage, stable, inexpensive, and reliable devices. The fundamental knowledge gained from this work will contribute to product development.

To establish high efficiency, low-voltage, stable materials for practical, organic light emitting diode based general illumination applications, it is necessary to simultaneously ensure that: essentially all electrons and holes injected into the structure form excitons; the excitons recombine radiatively with high probability; the minimum drive voltage is required to establish a given current density in the device; and the material and device are stable under continuous operation. We will apply a tightly knit theory/fabrication/ measurement approach to understand and optimize four essential material and device elements necessary for satisfying these requirements: 1) charge injection, 2) carrier mobility, 3) organic/organic heterojunctions, and 4) exciton processes. Because of the many material and device options available, we will develop general methods of achieving the device requirements in these four areas.

Keywords: Lighting, Light-Emitting Diodes, Organic Light-Emitting Diodes, Solid State Lighting

FENESTRATION MATERIALS DEVELOPMENT

5. 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 $520,000
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. Sage won a 100 R&D Award in 2004. Currently, Sage has constructed a new full scale production factory that will be capable of producing larger products. Research continues on improving the material coating process to increase production yields, and innovative production techniques to bring down the long term cost.

$500,000
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. LBNL won a 100 R&D Award in 2004.

In FY05, the main focus was to produce a first working prototype to demonstrate the technical viability of a novel design utilizing a hydrogen reservoir in combination with a simplified multilayer reflective device. Significant progress was made in improving both the cycling stability and switching range in gasochromically switched metal hydride films. This was done primarily by incorporation of a thin, transparent barrier layer that restricts interdiffusion of the palladium catalyst and the magnesium component of the optically active layer. While LBNL was successful in developing a prototype, the design had limited capability so full characterization and durability testing was not conducted.

DOE $200,000, Rockwell $50,000
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 small 100 cm^2 demonstration device was delivered in FY05 and will be characterized in terms of optical parameters (visible light transmission, reflectance and haze), mirror uniformity as a function of switching speed, and cycle life by NREL. This project is complete.

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

NEW BUILDING MATERIAL DEVELOPMENT AND HYGROTHERMAL MODELING

6. PHASE CHANGE MATERIAL (PCM)-ENHANCED CELLULOSE BASED INSULATION
   $150,000
   DOE Contact: Marc LaFrance, (202) 586-9142
   ORNL Contact: Andre Desjarlais, (865) 574-0022

The key task is to develop the next generation of low density cellulosic thermal insulation materials that would include a blending of a microencapsulated phase change material. If successful, this PCM-enhanced cellulose would perform as a massive building component because a thermal mass effect would be provided by specially tailored phase change material.

ORNL has demonstrated that encapsulated PCMs could be successfully blended into cellulose insulation with quantities up to 30% by weight added. Equipment and techniques were developed to accomplish this task. This addition was shown not to negatively impact the steady-state R-value of the insulation and did not compromise the fire resistance of the material. The blended insulation has been applied successfully to a test wall and attic assembly without PCM separation.

Keywords: Insulation, Phase Change Material, Cellulose

7. HYGROTHERMAL PROPERTY MEASUREMENTS & MODELING UPGRADES AND APPLICATIONS
   $423,000
   DOE Contact: Marc LaFrance, (202) 586-9142
   ORNL Contact: Andre Desjarlais, (865) 574-0022

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

Keywords: Hygrothermal, Phase Change Material, Moisture, Building Materials, Insulation, Heat-Air-Moisture, Material Properties

FREEDOMCAR AND VEHICLE TECHNOLOGIES PROGRAM

	FY 2005
FREEDOMCAR AND VEHICLE TECHNOLOGIES PROGRAM GRAND TOTAL	$36,477,000
TRANSPORTATION MATERIALS PROGRAM	$11,950,000
AUTOMOTIVE PROPULSION MATERIALS	$1,775,000
Low-Cost, High Energy Product Permanent Magnets	300,000
Characterization of Anisotropic Sintered Magnets	50,000
Graphite Foam Thermal Management Materials for Electronic Packaging	300,000
Mechanical Characterization of Electronic Materials and Electronic Devices	125,000
Microwave Regenerated Fiber Diesel Particulate Filter	75,000
Fabrication of Small Fuel Injector Orifices	250,000
Electrochemical NO_x Sensor for Monitoring Diesel Emissions	350,000
Hydrogen Compatibility of Materials for Automotive Applications	200,000
Advanced Materials Development Through Computational Design for HCCI Engine Applications	125,000
AUTOMOTIVE LIGHTWEIGHT MATERIALS (ALM)	$16,260,000
Automotive Metals	6,107,000
Polymer Composites Research and Development	4,589,000
Low-cost Carbon Fiber	1,717,000
Recycling	1,793,000
Joining	867,000
Non-destructive Evaluation	712,000
Materials Crosscutting R&d	475,000
HEAVY VEHICLE PROPULSION MATERIALS	$4,075,000
High-Toughness Materials	95,000
Materials for Exhaust Aftertreatment	250,000
Catalyst Characterization	200,000
Development of NO_x Sensors for Heavy Vehicle Applications	175,000
Electron Microscopy for Characterization of Catalyst Microstructures and Deactivation Mechanisms	190,000
Microstructural Changes in NO_x Trap Materials Under Lean and Rich Conditions at High Temperatures	95,000
Aftertreatment Catalysts Materials Research	0
Catalysts Via First Principles	300,000
Durability of Particulate Filters (Crada with Cummins, Inc.)	300,000
Lightweight Valve Train Components	150,000
Engineered Surfaces for Diesel Engine Components	75,000
Cermet Materials for Diesel Engine Wear Applications	40,000
Nanoengineered Materials	50,000
NDE of Diesel Engine Components	175,000
Durability of Diesel Engine Component Materials	180,000
Life Prediction of Diesel Engine Components	95,000
Low-Cost Manufacturing of Precision Diesel Engine Components	150,000
Advanced Machining and Sensor Concept	80,000
Advanced Cast Austenitic Stainless Steels for High-Temperature Exhaust Components	160,000
TiAl Nanolaminate Composites	5,000
Laser Surface Texturing of Lubricated Ceramic Parts	5,000
Low Cost Titanium Feedstock Consolidation Process	5,000
High Density Infrared Surface Treatment of Materials for Heavy-Duty Vehicles	70,000
High Temperature Aluminum Alloys	0

FREEDOMCAR AND VEHICLE TECHNOLOGIES PROGRAM (continued)

	FY 2005
HEAVY VEHICLE PROPULSION MATERIALS (continued)	
Titanium Alloys for Heavy-Duty Vehicles	95,000
Mechanical Behavior of Ceramic Materials for Heavy Duty Diesel Engines	275,000
Powder Processing of Nanostructured Alloys Produced by Machining	110,000
Deformation Processes for the Next Generation Ceramics	95,000
High Speed Machining of Titanium	75,000
Walker Process for Stress Relief	5,000
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	190,000
Testing Standards	75,000
IEA - Rolling Contact Fatigue	65,000
HIGH STRENGTH WEIGHT REDUCTION (HSWR) MATERIALS	$7,692,000
Application of Innovative Materials	1,116,000
Lightweight Vehicle Structures	2,046,000
Materials Processing Development	262,000
Materials Development	2,163,000
Enabling Technologies	2,105,000
HIGH TEMPERATURE MATERIALS LABORATORY	$6,100,000
High Temperature Materials Laboratory User Program	6,100,000
ELECTRIC VEHICLE R&D PROGRAM	$575,000
ADVANCED BATTERY DEVELOPMENT	$575,000
New High-Rate Electrode for Lithium-Ion Batteries	50,000
Binder- and Carbon-Free Oxide Electrodes for Diagnostic Studies	100,000
New High Energy Anodes for Improved Li Ion Batteries	75,000
Stabilization of High-Rate Mn Spinel Cathode Materials	100,000
Understanding Transport in Lithium Iron Phosphate	250,000

FREEDOMCAR AND VEHICLE TECHNOLOGIES PROGRAM

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

Within OFCVT, the bulk of the materials R&D is carried out through 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. The Electric Vehicle R&D program includes the support of Advanced Battery Development for electric and hybrid vehicle applications. The DOE contact is Tien Duong, (202) 586-2210.

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.

TRANSPORTATION MATERIALS PROGRAM

AUTOMOTIVE PROPULSION MATERIALS

8. 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 2005, we modified the existing 5/8-in. die and punch set to alleviate the trapped air problem during compact press. To allow air to escape more easily during compact pressing, it was decided to cut six flats (0.192-in. wide and 60 degrees apart) along the axial direction of the punch and a 0.20-in.-wide circular groove near the face of the punch. This design will reduce the resistance to air flow and still maintain relatively tight clearance between the die and punch during compact pressing. We fabricated 10 compacts using the new punches, all at a magnetic field of 2 Tesla to determine if there is any improvement in processing the compacts. We observed that the pressurization rate of the compact can be increased significantly over that of previous compacts made by using the original punches. We also noticed that pressure fluctuations were reduced during early stage of the pressing. These observations clearly indicate qualitatively that air was able to escape faster and easier from the die because the resistance for air flow is reduced.

In the past, powdered compacts frequently cracked during ejection from the die. In order to improve the success rate of compact ejection, a new die and punch set was fabricated by Bronson and Bratton, Inc. The thickness of the compact is 0.235 in. (5.969 mm) and the diameter of the compact changes from 0.6250 in. to 0.6293 in. (15.875 mm to 15.984 mm) continuously over the thickness of the compact. These dimensions are based on previous experience that the average diameter of the compact increased from 0.625 in. to 0.6290 in. (15.875 mm to 15.977 mm) during ejection from the die. The slightly tapered design is supposed to reduce the friction during compact ejection, which may alleviate the cracking problem encountered previously. We fabricated about a dozen compacts under different magnetic fields. We have 100% success and not a single compact cracked during and after ejection from the die. The results are very encouraging. In addition to alleviating the cracking problem using this tapered die and punch set, we were able to increase further the rate of pressurization during compact pressing without causing cracks in the ejected compact.

In FY 2005, the preliminary report on the economic study submitted by Data Decisions was revised based on the comments received from DOE, ANL, and ORNL. The report is being finalized and will be issued in FY 2006.

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

9. CHARACTERIZATION OF ANISOTROPIC SINTERED MAGNETS
$50,000
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 utilized in the drive motor and dozens of actuators in electric vehicles offers an opportunity for significant weight reduction. At ORNL, work has been carried out to characterize sintered and bonded magnets fabricated under different conditions. In particular, work has been focused to assess the effect of grain size, texture, composition and impurity phases on the magnetic properties of sintered and bonded magnets.

During FY04, a test facility was designed and built to investigate the effects of thermal cycling on both the mechanical and magnetic properties of sintered and bonded magnets. Preliminary tests have been carried out between –40˚C and 150˚C, which is the range of temperatures that permanent magnets will experience in automotive applications. The experimental set-up allows for the determination of changes in the magnetic strength of magnets as a function of temperature and time, while mechanical properties (e.g., elastic properties, mechanical strength) are determined at the end of thermal cycling tests.

During FY04 a collaboration was established with IAP (Dayton, OH), to evaluate permanent bonded magnets densified according to IAP's patented dynamic magnetic compaction process. During FY05, collaborative efforts with IAP, Argonne National Laboratory and Ames National Laboratory continued to characterize magnets synthesized at these three sites, in particular to assess the effects of thermal cycling on their mechanical and magnetic properties.

Keywords: NdFeB, Permanent Magnets

10. 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 cooling inverters in order 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 increased by an order of magnitude compared to traditional materials and designs. A mathematical model was developed to predict the thermal performance of the foam in heat sink applications. However, the current model needs to be expanded to relate materials parameters (i.e., materials optimization) to the thermal properties for use in a power electronic thermal management system.

Collaborative work with Ford Motor Co. will continue to evaluate and optimize carbon foam for cooling of power electronics of Ford's Hydrogen Hybrid Research Vehicle (H2RV). Conventional heat sinks designs and alternative cooling techniques will be evaluated.

In order to capitalize on the modeling effort, work will continue on understanding how thermal conductivity and foam microstructure are affected by processing conditions in order to optimized foam properties for a given application. Work will also be conducting on characterizing the interface of the foam with different bonding techniques, by measuring the temperature drop across the interface using micro thermocouples and well as a high-speed infrared camera calibrated with the micro thermocouples.

Carbon foam has shown great potential for use in passive cooling techniques such as evaporative cooling. Work will be directed to explore in more details this application. We will study the role of foam properties and structure as well as the role of the evaporant on thermal transfer. Partnership with a commercial manufacturer or end user will be necessary in order to correctly address the critical needs for a given 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

11. MECHANICAL CHARACTERIZATION OF ELECTRONIC MATERIALS AND ELECTRONIC DEVICES
$125,000
DOE Contact: R. 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

12. MICROWAVE REGENERATED FIBER DIESEL PARTICULATE FILTER
$75,000
DOE Contact: R. Sullivan, (202) 586-8042
ORNL Contact: D. P. Stinton, (865) 574-4556
Industrial Ceramic Solutions Contact: R. Nixdorf, (865) 482-7552

The current accepted diesel particulate filter solution is based upon an extruded ceramic honeycomb design, similar to catalytic converters that have been installed on American automobiles since the mid-1970s. This design works on large diesel engines, such as highway transport trucks, where exhaust temperatures are high enough to allow catalyst coatings to burn trapped particulate matter and keep the filters clean. There are millions of smaller diesel engines that require auxiliary exhaust heating to clean the filter during engine operation. ICS has developed a pleated ceramic fiber filter cartridge that is especially suited for the lower exhaust temperatures in smaller engines. This cartridge removes more than 95% of diesel soot particles. Its greatest advantage is the fact that it filters at a fraction of the backpressure exerted on the engine compared to competitive products.

Backpressure on a diesel engine reduces the efficiency of the engine and increases the fuel consumption penalty caused by an obstruction in the exhaust system. The backpressure of the ICS fiber filter is one-tenth that of the extruded honeycomb filter product. In addition, the thermal mass of the ICS filter is one-third that of the honey-comb filter. This means that it requires less auxiliary energy to achieve filter cleaning, again reducing the fuel penalty for the emission control device. These advantages can reduce the fuel consumption penalty from 15% to 1%. The final advantage is the cost of the product in a high-volume market. The simple pleated design is similar to that of millions of air and liquid filtration devices used around the world. It is manufactured by established processes on high-volume equipment.

FY 2004 accomplished the completion of the prototype fabrication and vehicle testing of the Round Pleated Ceramic Fiber Filter. The FY 2005 work focused on optimizing the Round Pleated Filter cartridge for the U.S. automotive market manufacturer's testing. This optimization program will produce various sizes and shapes to provide suitable test filter cartridge samples to the heavy-duty truck, heavy-duty pickup, light-duty pickup and SUV, off-road stationary, and diesel retrofit markets. The milestone for the program will be the supply of prototype test cartridges to at least one customer in each of these categories.

Keywords: Carbon Particulates, Diesel, Filters, Microwave Regeneration

13. FABRICATION OF SMALL FUEL 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 be used to fabricate orifices as small as 100 mm in diameter. Ideally, however, the orifice diameter should be reduced to 75 mm or less. While laser percussive drilling can readily achieve these diameters with very short process times, the heat-affected zone around the orifice fails rapidly in use due to its brittleness. 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 with electroless nickel plating demonstrated the ability to reduce the diameter of 200 mm diameter orifices down to 50 mm. The process has been transferred to a commercial coating company, and efforts are underway to prepare nozzles for fuel spray and engine emission studies by machining away some of the plating. We are also continuing studies of deposit formation on coatings of various compositions, to determine the impact of the coatings on deposit formation and possibly engineer the coating composition to reduce or eliminate nozzle blockage by deposit formation. As part of these studies we are testing bioderived lubricants as surrogates for biodiesel. In 2005 we initiated an examination of the cavitation erosion resistance of different electroless nickel compositions, as a means of evaluating the durability of plated nozzles.

Keywords: Fuel Injectors, Nozzles, Orifice, Coating

14. ELECTROCHEMICAL NO_X SENSOR FOR MONITORING DIESEL EMISSIONS
    $350,000
    DOE Contact: R. A. Sullivan, (202) 586-8042
    LLNL Contact: R. S. Glass, (925) 423-7140
    LLNL Principal Investigators: R. S. Glass and 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 Innovation and Research Center 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 the exploration of novel, impedance-based sensing methodologies which have recently been observed to exhibit promising performance. Operating parameters including temperature, frequency, excitation voltage, and electrode microstructure are being evaluated. Additionally, techniques for compensating the O_2 and temperature response of the sensor are being developed.

Keywords: NO_x, Electrochemical Sensor, CIDI, Diesel Exhaust

15. HYDROGEN COMPATIBILITY OF MATERIALS FOR AUTOMOTIVE APPLICATIONS
    $200,000
    DOE Contact: R. A. Sullivan, (202) 586-8042
    ORNL Contact: D. P. Stinton, (865) 574-4556
    PNNL Contact: James Holbery, (509) 375-3686

This research effort aims to better understand and quantify the function and durability of both actuator and injector materials considered for direct inject hydrogen internal combustion engine (H-ICE) application. The development of 100% hydrogen high pressure exposure chambers combined with in-situ test capabilities has established PNNL with unique material test capabilities for hydrogen service within the DOE Laboratory system. This effort is supported by atomistic models developed to quantify the diffusion of high pressure hydrogen into solids; our objective is to connect the nano-to-macro scale effects of hydrogen on solid material durability and performance.

Current efforts include the following:

- Conduct H-ICE injector and actuator failure analysis.
- Measure the performance of actuators and actuator materials in high pressure, high temperature 100% hydrogen environments.
- Evaluate in-situ and ex-situ injector material wear, actuator performance, and impact behavior to quantify and predict long-term material durability.
- Develop models to predict hydrogen diffusion into solids, including piezo materials.

Keywords: Hydrogen, H-ICE, Injector Materials

16. ADVANCED MATERIALS DEVELOPMENT THROUGH COMPUTATIONAL DESIGN FOR HCCI ENGINE APPLICATIONS
    $125,000
    DOE Contact: R. Sullivan, (202) 586-8042
    ORNL Contact: D. P. Stinton, (865) 574-4556
    ORNL Principal Investigator: V. K. Sikka, (865) 574-5112

There has been an increasing interest in homogeneous charge compression ignition (HCCI) combustion in recent years because of its potential to increase engine combustion efficiency and reduce emissions. However, the use of the HCCI combustion concept will subject the engine components to significantly higher temperatures and pressures. The temperatures for diesel engines will reach over 1600°F and pressure may reach > 2000 psi, which is approximately four times that of the normal combustion engine. Such severity in engine operating conditions will require a significant improvement in the materials performance in order to take advantage of the HCCI engine concept. This project deals with identifying materials requirements for HCCI engines for automotive and truck applications and the development of advanced, yet cost effective materials through computational design.

Seven automotive and truck companies were contacted. Based on discussions with these companies, four improved materials needs and opportunities have been identified in support of advanced engine concepts such as HCCI.

1. Optimization of Ni alloys for exhaust valves to reduce cost, extend high-temperature performance, and improve high-temperature fatigue life.
2. High-strength, thermally, corrosion-resistant aluminum for charge air coolers.
3. For cast irons, effect of alloying elements on cost, high-temperature capability, and greater crack resistance under temperature and stress cycling.
4. Wear-resistant, higher strength, higher temperature, capable alloy steels for fuel injection components.

As a first step to materials development through computational design approach, phase equilibrium calculations were carried out on published candidate compositions of Ni-based alloys for exhaust valves. The alloys used for calculations were 70Ni-19Cr, IN751, and Nimonic 90A.

Initial calculations of materials development through computational design were completed for three published Ni-based alloy compositions. The weight percent of g¢ phase shows a qualitative agreement with the published fatigue data on two of the three alloys used in the calculations.

Keywords: HCCI, Advanced Engine Materials

AUTOMOTIVE LIGHTWEIGHT VEHICLE MATERIALS

17. AUTOMOTIVE METALS
    $6,107,000
    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, Lawrence Livermore National Laboratory, Sandia National Laboratory
    Industry Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors), American Iron and Steel Institute, Ispat Inland, US Steel, Roman Engineering, Dofasco, Stelco, Westmoreland, Tribsys Inc., Altair Engineering, Magna International, American Foundryman's Society, Stackpole Ltd., Valimet, Aluminum Consultant's Group, Eck Industries, Meridian, Spartan Die Casting, Lunt Industries.
    University Partners: Oakland University,

University of Toledo, University of Missouri, University of Dayton Research Institute, Georgia Tech, Mississippi State University, University of Kentucky, University of Tennessee

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 evaluate new low-cost titanium powders, to develop capabilities for designing with advanced high strength steels and to evaluate technologies for forming them. Activities also 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; 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 cast magnesium alloys in place of aluminum in structural components and powertrain applications.

Keywords: Aluminum, Sheet Forming, Warm Forming, Hydroforming, Electromagnetic Forming, Titanium, Magnesium, Advanced High Strength Steels, Stamping, Casting, Powder Metallurgy, Crashworthiness, Springback, Tribology, Numerical Modeling, Die Casting

18. POLYMER COMPOSITES RESEARCH AND DEVELOPMENT
    $4,589,000
    DOE Contact: Joseph Carpenter, (202) 586-1022
    ORNL Contact: Phil Sklad, (865) 574-5069; Dave Warren, (865) 574-9693
    Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory
    Industrial Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors)
    University Partners: University of Tulsa, South Dakota School of Mines, University of Michigan-Dearborn

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. Other activities focus on crash energy management of composite materials, durability of composites, and modeling and simulation of polymer composite processing and performance.

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

19. LOW-COST CARBON FIBER
    $1,717,000
    DOE Contact: Joseph Carpenter, (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069, 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, Westvaco, Hexcel Corp.

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, Processing, Low Cost Carbon Fiber, Microwave Processing, Precursors

20. RECYCLING
    $1,793,000
    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 other lightweight materials, to establish priorities for advanced recycling initiatives and provide technical oversight to ensure that priority goals and objectives are accomplished.

Keywords: Recycle, Polymer Composites

21. JOINING
    $867,000
    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)
    University Partners: University of Michigan

The objective of this effort is to develop technologies that remove barriers to implementation of lightweight materials in automotive applications. In particular, 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; 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, Numerical Modeling, Friction Stir Spot Welding

22. NON-DESTRUCTIVE EVALUATION
    $712,000
    DOE Contact: Joseph Carpenter, (202) 586-1022
    ORNL Contact: Phil Sklad (865) 574-5069
    LLNL Contact: Jim Prindeville, (925) 422-3169
    Laboratory Partners: Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory
    Industry Partners: United States Automotive Materials Partnership (DaimlerChrysler, Ford, General Motors)

The objective of this effort is to evaluate or develop advanced non-contact non-destructive evaluation technologies which have the potential for realtime measurements in the manufacturing environment. 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.

Keywords: Development of Non-Destructive Evaluation Equipment, Procedures, Process Sensors

23. MATERIALS CROSSCUTTING R&D
    $475,000
    DOE Contact: Joseph Carpenter, (202) 586-1022
    ORNL Contact: Phil Sklad, (865) 574-5069
    PNNL Contact: Mark Smith, (509) 375-4478
    Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory

The objective of this effort is to develop crosscutting technologies which allow cost and production efficient incorporation of advanced materials into automotive components. This activity also provides the evaluation tools necessary to asses the current and potential effectiveness of the research portfolio. Some projects focus on developing standard test and evaluation methodologies and comprehensive design models.

Keywords: Cost Modeling, Crashworthiness, Structural Reliability, Glazing

HEAVY VEHICLE PROPULSION MATERIALS

24. HIGH-TOUGHNESS MATERIALS
    $95,000
    DOE Contact: James J. 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_{Ic}) 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. The activities in FY 2005 will complete the support effort for the TiC-Ni_3Al components for diesel fuel injection systems that is done in conjunction with both CoorsTek (parts producer) and Cummins Engines (engine manufacturer).

TiAl offers significant improvements in weight-to-strength ratios compared to most advanced alloys. Such materials could have applications in heavy vehicle propulsion systems. Ceramic-metal composites that utilize TiAl as the bonding phase potentially could show increased fracture strength, higher elastic modulus, better creep resistance and higher wear resistance than the base alloy. An exploratory study will be initiated to fabricate ceramic particulate reinforced TiAl composites and determine the mechanical properties. Initial samples will be fabricated by hot-pressing to readily obtain high density specimens suitable for testing. An assessment will be made to determine if the mechanical properties are suitable for further development for heavy vehicle applications.

Keywords: Cermets, NiAl, TiC

25. MATERIALS FOR EXHAUST AFTERTREATMENT
$250,000
DOE Contact: James J. Eberhardt, (202) 586-9837
ORNL Contact: D. R. Johnson, (865) 576-6832
Caterpillar Contact: Craig Habeger, (309) 578-4468

NO_x sensor- Further research will focus on alternative technologies for sensing NO_x in the diesel exhaust environment. The primary focus will be developing sensors based on metalloporphyrines chemistry. The program will focus on identifying porphyrine compounds that will survive and behave predictably in the exhaust environment. The computational modeling that started in the 4Q04 will be completed in FY05. The NO_x concentrations are creeping down below the limits of current sensor technologies and a NO_x sensor may need to measure reliably below 5 ppm NO_x. The porphyrine-based sensors will focus on sensing near 1 ppm NO_x. The program approach will be as follows with a goal of identifying a production-suitable sensor: define suitable porphyrine molecules to bind NO_x using computational modeling, initial evaluation of porphyrine molecules to detect NO_x in limited bench experiments, utilize bench tests to determine the effects of gas composition, temperature, pressure on sensor accuracy, repeatability, and response time.PM Trap-This project will continue to focus on understanding physical and chemical properties of soot, and understanding the soot interaction with PM filters and catalyzed PM filters. This project will also focus on developing materials and designs for diesel particulate trapping applications. The trapping technologies will be evaluated for filtration efficiency using the diesel fuel burner. The ability to catalyze the new designs will also be evaluated. In addition, evaluation of the state-of-the-art PM removal technologies will be performed using a diesel burner.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

26. CATALYST CHARACTERIZATION
$200,000
DOE Contact: James J. 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 FY04 effort, rates of desulfation and activation energies for various catalytic compositions after different periods of aging were obtained via spectroscopy. Characterizations continued for new materials from various stages of the catalyst’s lifecycle. E*x-situ* microchemical and crystallographic studies of these new materials in simulated engine environments were conducted.

Keywords: NO_x, SCR, Sensors, Exhaust Aftertreatment

27. DEVELOPMENT OF NO_X SENSORS FOR HEAVY VEHICLE APPLICATIONS
$175,000
DOE Contact: James J. Eberhardt, (202) 586-9837
ORNL Contact: D. R. Johnson, (865) 576-6832

Combustion of low-sulfur fuel results in three main pollutants: CO, hydrocarbons (HC), and oxides of nitrogen (NO_x, a mixture of NO and NO_2). Fuel-injected, spark-ignited engines for passenger cars currently employ a three-way catalyst (TWC) to greatly reduce the levels of these three pollutants. Unfortunately, the TWC can only remove all three pollutants within a narrow range of oxygen concentrations in the exhaust, losing its effectiveness for NO_x removal at higher O_2. Therefore this TWC cannot be employed for NO_x remediation of exhausts from diesel and lean-burn gasoline engines, as these tend to be O_2-rich.

Two methods are being developed to reduce NO_x emissions: 1) a NO_x trap and 2) selective catalytic reduction. For selective catalytic reduction the amount of reagent injected is critical, as enough must be supplied to completely decompose the NO_x, but the addition of excess must be avoided. Therefore it is essential to develop sensors that can rapidly and accurately assess the NO_x levels in these exhausts and enable improved emissions control and on-board diagnostics. NO_x traps adsorb the NO_x in the exhaust gas stream and then decompose it catalytically with a soft plasma, when the trap reaches a threshold level. NO_x sensors are required to determine when the NO_x trap become full and needs to regenerate. A suitable sensor would be operative at T ~700^{o}C and able to measure NO_x in the range 1-1000 ppm.

This project seeks to develop and characterize NO_x *sensing elements* (for incorporation into working sensors) targeted to meet the demands outlined above. The elements consist of co-planar oxide and noble metal electrodes on an oxygen-ion conducting substrate. Similar material combinations have been used in “potentiometric” NO_x sensing devices, but in the present investigation we do not employ a reference electrode, thus simplifying the sensor design.

In FY 2003 and FY 2004 the first fully operational NO sensor was developed and tested. Using a current bias, this sensor demonstrated the ability to accurately detect NO over the range 1 to 1000 ppm with a response time of 1-2 seconds at 550˚C. This sensor has subsequently been tested at Ford Motor Co. and shown to have little or no sensitivity to hydrocarbons and carbon monoxide. It does, however, have a measurable sensitivity to ammonia and steam. While this is a breakthrough in NO sensing technology work is still required to optimize the electrode design, structure, and composition. Further, additional testing is required to fully understand the operational sensitivities of this novel sensor system in both simulated and real exhaust gas environments. Therefore, in FY 2005 work will continue with increased activities focused on developing novel sensor electrode configurations, and testing to ascertain steam and ammonia. In addition, development of the electrode materials will continue to modify composition and morphology to optimize sensor performance. Studies will also be implemented to use impedance spectroscopy and temperature programmed desorption to understand the reaction mechanisms taking place at the electrode surfaces.

Keywords: Sensors, NO_x, Exhaust Aftertreatment

28. ELECTRON MICROSCOPY FOR CHARACTERIZATION OF CATALYST MICROSTRUCTURES AND DEACTIVATION MECHANISMS
    $190,000
    DOE Contact: James J. 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 that will achieve beneficial operation by the beginning of FY2005, will be exploited to provide the highest resolution imaging and spatial resolution energy-loss spectroscopy in the world.

The objective of the proposed research is to continue 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 (Dr. Stewart Daw) and both model and “real” catalysts for NO_x trapping applications with Ford Research Laboratory (Dr. George Graham)] so that the catalytic performance can be improved further through a proper design of catalyst preparation processes or an addition of necessary catalytic “promoters.” Ultra-high resolution dark-field imaging (i.e. "Z-contrast" scanning transmission electron microscopy with the ACEM) will be combined with energy-loss spectroscopy to determine the effects of aging on the surface structure and dispersion of heavy metal species on oxide supports.

Keywords: TEM, Catalyst, Microstructure

29. MICROSTRUCTURAL CHANGES IN NO_X TRAP MATERIALS UNDER LEAN AND RICH CONDITIONS AT HIGH TEMPERATURES
$95,000
DOE Contact: James J. Eberhardt, (202) 586-9837
ORNL Contact: D. R. Johnson, (865) 576-6832

We recently completed microstructural analysis on NO_x traps from (1) Ford supplier that were aged on a pulsator at Ford and (2) Ford DISI fleet in Europe after 30,000 and 82,000 km. The pulsator aged lean and rich aged samples showed that the sintering of platinum particles occurs during aging and barium migrates into ceria-zirconia layer. Both of these factors reduce platinum-barium oxide surface area where NO_x adsorption and reduction takes place during lean and rich cycles respectively. The stoichiometric aging also leads to the migration of barium into ceria-zirconia layer but the sintering of platinum is less severe. On vehicle aged samples show rapid sintering of Pt particles to about 15 nm after only 30,000 km. These studies combined with our earlier study of microstructural changes in NO_x trap materials after aging on a dyano completes a base-line for determining the ability of bench flow reactor and dyano to duplicate on-vehicle aging of NO_x traps.

We updated the *ex-situ* reactor at ORNL to enable the control of diesel and gasoline lean and rich (simulated) environments. Our preliminary studies of microstructural changes in NO_x trap materials at 500ºC using an ex-situ reactor that is capable of maintaining either lean, rich, or stoichiometric environment shows that aging experiments of bench-flow reactors can be reproduced on the ex-situ reactor. This suggests that ex-situ reactor can be used a high-throughput screening tool. We are further updating this reactor to make it capable of lean-rich cycling and we anticipate establishing ex-situ reactor as a high throughput screening tool for studying the microstructural changes in a variety of catalyst materials and co-relating them with aging.

We have completed the study of microstructural changes in model NO_x trap materials Pt/[10%CeO_2-ZrO_2-90%(3%La_2O_3-97%BaO.6Al_2O_3)] under lean and rich conditions, at 500ºC for 4 hours using ex-situ reactor. The results are identical to the ones observed using bench-flow reactor. We also analyzed bench-flow reactor samples using techniques of electron microscopy, X-ray analysis and surface analysis. We plan to complete this study at 900ºC. Furthermore, we want to incorporate SO_2 in our simulated exhaust to study its impact on microstructural changes. We then plan to study the changes under lean-rich cycle conditions. Based on our early the results, we have prepared new model materials, Pt-MnO_2/[10%CeO_2-ZrO_2-90%(3%La_2O_3-97%BaO.6Al_2O_3)] to study the impact of MnO_2 in reducing Pt sintering. We plan to 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

30. AFTERTREATMENT CATALYSTS MATERIALS RESEARCH
$0
DOE Contact: James J. 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: abatement of diesel soot and reduction of NO_x:

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

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

31. CATALYSTS VIA FIRST PRINCIPLES
$300,000
DOE Contact: James J. 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 CO oxidation reactions.

Keywords: Catalytic Materials, Catalytic Testing, Experimental Catalysis

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

In collaboration with researchers at Cummins Inc., probabilistic models will be developed to predict the reliability and durability of ceramic Diesel Particulate Filters (DPF). These modeling efforts will account for the meso-structure of the DPFs and will be complemented with experimental activities to determine their physical and mechanical properties. In turn, experimental results will be used as input for the probabilistic models. In particular, methodologies will be developed and implemented to determine the distribution of strengths of DPFs, and the evolution of their elastic properties and crack-growth resistance with time.

Keywords: Diesel, Particulates, Filters, Ceramic Substrates

33. LIGHTWEIGHT VALVE TRAIN COMPONENTS
    $150,000
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    Caterpillar Contact: Jeremy Trethewey,
    (309) 578-0056

Valve train components in heavy-duty engines operate under high stresses and temperatures, and in severe corrosive environments. In contrast, the valve train components in the light-duty engine market requires cost-effective reliable materials that are wear resistant and lightweight in order to achieve high power density. For both engine classes, better valve train materials need to be identified to meet market demand for high reliability and improved performance while providing the consumer lower operating costs. Advanced ceramics and emerging intermetallic materials are highly corrosion and oxidation resistant, and possess high strength and hardness at elevated temperatures. These properties are expected to allow higher engine operating temperatures, lower wear, and enhanced reliability. In addition, the lighter weight of these materials (about one-third of production alloys) will lead to lower reciprocating valve train mass that could improve fuel efficiency. This research and development program is an in-depth investigation of the potential for use of these materials in heavy-duty engine environments. The overall valve train effort will provide the materials, design, manufacturing, and economic information necessary to bring these new materials and technologies to commercial realization. With this information, silicon nitride and titanium aluminide valve designs will be optimized using computer-based lifetime prediction models, and validated in rig bench tests and short-and long-term engine tests.

Keywords: Valves, Diesel Engines, Life Prediction

34. ENGINEERED SURFACES FOR DIESEL ENGINE COMPONENTS
    $75,000
    DOE Contact: James J. 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

35. CERMET MATERIALS FOR DIESEL ENGINE WEAR APPLICATIONS
    $40,000
    DOE Contact: James J. 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

36. NANOENGINEERED MATERIALS
    $50,000
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    ORNL Contact: D. R. Johnson, (865) 576-6832
    NCA&T Contact: Jag Sankar, (336) 256-1151

In our present research NCA&T is fabricating anode and cathode substrates using slip casting and sintering. In FY 2005, we will continue this work to produce large area anode and cathode substrates. By optimizing the material composition and processing variables, we will make substrates with satisfactory microstructures and improve their mechanical and electrical properties. We will produce electrolyte thin film coating on one of these substrates by three methods, i.e. combustion chemical vapor deposition, electrolytic deposition, and electrophoretic deposition. We will also make single fuel cell at the end for demonstration and testing.

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

37. NDE OF DIESEL ENGINE COMPONENTS
    $175,000
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    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 induced damage in structural ceramic valves for diesel engines using various nondestructive evaluation (NDE) methods. The primary NDE method is elastic optical scattering or laser scattering which has been demonstrated capable of detecting fracture origins and damage type and intensity. The goal is to establish this method so it can be reliably used to determine subsurface defects/damage microstructure as well as to predict mechanical properties for silicon nitride ceramics. There are two tasks to be completed: (1) Characterize subsurface defects and damage induced by machining or mechanical testing and correlate NDE data with microstructural and mechanical properties for several candidate silicon nitrides selected for valves. (2) Assess initial quality and 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

38. DURABILITY OF DIESEL ENGINE COMPONENT MATERIALS
    $180,000
    DOE Contact: James J. 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. A test method was developed to study the friction and wear characteristics of candidate exhaust gas recirculation (EGR) system materials. Selected commercial alloys, ceramics, and experimental materials were evaluated for their high-temperature (650^{o}C) scuffing behavior. In FY 2002, an investigation was begun into the basic causes for scuffing in fuel injector component materials. Testing techniques were developed to replicate the surface damage mechanisms characteristic of diesel engine fuel system parts. The effects of sulfur content in the diesel fuel on scuffing were evaluated, and tests were conducted to evaluate the scuffing behavior of both intermetallic alloy-based cermets and traditional hard coatings in fuel environments. A new technique was developed to detect the early stages of scuffing. Contact damage evolution in ceramics and metals for high-temperature scuffing applications was studied using a state-of-the-art scanning acoustic microscope. In FY 2004, multi-dimensional, graphical depictions were developed to portray the evolution of scuffing damage in boundary-lubricated tribosystems. Detailed scanning electron microscope observations were correlated with transitions in frictional behavior.

In FY 2005 an analytical model for selecting materials for scuffing-critical applications will be developed and validated experimentally. Also in FY 2005, a new task will be undertaken to engineer the surfaces of titanium alloys to make them more suitable in friction and wear sensitive engine components such as pistons. Surface engineering methods like laser dimpling and thermal treatments will be employed to overcome some of the friction and wear limitations exhibited by as-cast titanium alloys.

Keywords: Tribology, Friction and Wear, Scuffing

39. LIFE PREDICTION OF DIESEL ENGINE COMPONENTS
    $95,000
    DOE Contact: James J. 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. In FY04 efforts on generation of mechanical database for new candidate silicon nitrides, manufactured by domestic suppliers, were continued. Evaluation of mechanical properties and microstructure of NT551 silicon nitride valves after 500-h bench rig test was also accomplished. In FY05, efforts on database generation for specimens machined from SN235P silicon nitride valve stems will be initiated. Also, characterization of mechanical properties and microstructure of SN235P silicon nitride valves will be carried out after engine test at NTRC.

Keywords: Life Prediction, Mechanical Characterization

40. LOW-COST MANUFACTURING OF PRECISION DIESEL ENGINE COMPONENTS
    $150,000
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832

Cost-effective machining processes are needed to make possible the widespread use of high-performance materials in engine components. By optimizing the use of high-performance material properties during the design process, components such as fuel injectors, valves, valve guides, cam rollers and EGR parts can be made from structural ceramics, ceramic-composites, and intermetallic alloys. ORNL has equipped its machine tools with instrumentation for studying the fundamentals of machining processes needed to make precision components from these materials.

In FY 2004, this effort was refocused on the cost-effective machining of next-generation of light weight diesel engine materials. This was a change from ORNL's historical focus on the machining of ceramics toward other engine materials of current interest, such as titanium and composite materials based on metals and ceramics. Starting in FY 2004, a new collaboration with Third Wave Systems, Minneapolis, MN, is providing an in-house capability to model high-speed machining of titanium alloys and other difficult-to-machine materials like metal matrix composites. In addition, increased emphasis will be placed on the response of materials to the machining processes. That approach will draw on ORNL's traditional strengths in material characterization to link machining and finishing process parameters with surface quality and ultimate functionality. In FY 2005, plans are to conduct a systematic study of the machining characteristics of advanced cermet materials that were specially-produced with variations in the reinforcing particle concentration.

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

41. ADVANCED MACHINING AND SENSOR CONCEPT
    $80,000
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832
    Univ. of Michigan Contact: Albert Shih,
    (919) 515-5260

The goal of this task is to advance enabling technologies for the cost-effective machining of Ti alloys. New Ti machining models, collaborating with the Third Wave Systems, will be implemented. Machining experiments, particularly the drilling and turning processes commonly used in heavy vehicle production, will be conducted to validate simulation results and evaluate new tool materials and coatings. Kennametal and ORNL are two collaborators in tool materials and coatings development. Diffusion wear is a predominate mode of tool wear in machining of Ti due to the high tool temperature. New TiC-NiAl cermet for tool material will be investigated. The measured tool wear will be quantitatively compared with modeling results.

Keywords: EDM, Temperature Measurement, Titanium

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

The objective of this follow-on second CRADA project between ORNL and Caterpillar is commercial scale up of the new modified cast austenitic stainless steels developed jointly as cost-effective, high-performance alternatives to 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 550-600^{o}C. While two new modified stainless steels were developed and tested (CF8C Plus and CN12 Plus), CF8C-Plus was found to have the best combination of as-cast ductility and strength, and high temperature aging, creep, fatigue and thermal-fatigue resistance, and to be far better than standard CF8C steel at 700-850^{o}C. The thermal fatigue resistance is essential for resistance to cracking during the severe thermal cycling that exhaust components experience. Last year, the new CF8C-Plus won a 2003 R&D 100 Award for outstanding properties performance and commercial scale up. Commercial scale up and testing continued this year, with creep, fatigue and thermal fatigue at 700-850^{o}C, long term aging and microcharacterization. This year, testing at ORNL and Caterpillar will be completed to provide the comprehensive properties data that is allowing designers to qualify these new alloys, and optimize component designs. This year, efforts to produce prototype diesel turbocharger components will begin, and efforts to expand the licensing and applications opportunities will continue. Long-term aging, creep testing, microcharacterization analysis, and casting of additional commercial heats of CF8C-Plus should be completed. This second advanced diesel engine CRADA (Cooperative Research and Development Agreement) project (ORNL 02-0658) was begun for a three-year period on July 21, 2002, and should be extended. More detailed information on this project must be requested directly from Caterpillar, Inc.

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

43. TiAl NANOLAMINATE COMPOSITES
    $5,000
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832
    LLNL Contact: Luke Hsiung, (925) 424-3125

In FY 2005, hot-extrusion processing techniques will continue to be utilized to fabricate a new class of TiAl-Ti_3Al nanolaminate composites with the addition of high alloying content of W (1 at. %) or Nb (>10 at. %), which is anticipated to enhance the high-temperature creep and oxidation resistance of the composite. Quench and age experiments will also be exploited to modify and refine the microstructure. Effort will be placed upon investigating the interrelationships between process parameters (extrusion ratio, temperature, and alloying additions) and microstructures (lamella thickness, dislocation structure, and interfacial substructure) of the laminate composite using optical metallography and transmission electron microscopy (TEM). Creep resistance and thermal stability of the nanolaminate composites at elevated temperatures up to 850°C will be measured and characterized.

Keywords: Titanium, Titanium Aluminide, Lamellar Microstructure

44. LASER SURFACE TEXTURING OF LUBRICATED CERAMIC PARTS
    $5,000
    DOE Contact: James J. 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 in reducing the friction of lubricated ceramic surfaces. Surface Technologies Ltd. has developed a laser-based method to prepare surfaces with arrays of microscale dimples, typically ~120 mm in diameter and several micrometers deep, spaced in rows about 100-200 mm apart. Under certain contact conditions, these regularly-spaced cavities in the surface can improve the ability of a flowing liquid lubricant film to support the bearing load. Research by other investigators has shown that the pattern density and the dimple shapes and orientations with respect to the flow direction can alter the magnitude of friction reduction.

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. 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 FY 2004, focused ion beam micro-sectioning methods were used to cut slivers from the bottoms of dimples in TTZ and to study, by high-resolution transmission electron microscopy and electron diffraction, the changes in their fine-structure resulting from rapid heating and cooling. In reciprocating tests, it was found that dimpling reduced friction only under well-aligned contact conditions and at higher rates of sliding. However, not all experimental results indicated improvements from laser dimpling.

In FY 2005, the ability to use laser dimples to supply solid lubricants to ceramic surfaces will be examined. With liquid lubrication, dimpling effects are primarily fluid dynamic, but there are two other uses of dimples in bearings: their ability to trap abrasive wear particles and their ability to serve as a lubricant reservoir. These additional aspects will be explored in FY 2005 using solid lubricants such as graphite.

Keywords: LST, Laser Surface Texturing

45. LOW COST TITANIUM FEEDSTOCK CONSOLIDATION PROCESS
    $5,000
    DOE Contact: James J. 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, vacuumsintering 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

46. HIGH DENSITY INFRARED SURFACE TREATMENT OF MATERIALS FOR HEAVY-DUTY VEHICLES
    $70,000
    DOE Contact: James J. 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. Previous work examined the processing parameters required to obtain uniform, adherent coatings on cast iron, low alloy steel, and tool steel. Initial wear testing showed improved wear resistance for the HDI coated materials. The activities for FY 2005 will examine the relationships between processing parameters, microstructural development, and wear resistance.

Keywords: Infrared Processing, Surface Treatment

47. HIGH TEMPERATURE ALUMINUM ALLOYS
    $0
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832
    Cummins Contact: Randy Stafford, (812) 377-3279

This work is directed at developing advanced high temperature aluminum alloys for turbocharger compressors and cost-effectively-produced, wear-resistant and nonmagnetic cermet materials for advanced fuel systems for diesel engine applications.

Keywords: Aluminum, Creep, Low-Cycle Fatigue

48. TITANIUM ALLOYS FOR HEAVY-DUTY VEHICLES
    $95,000
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832

Task 1: Titanium alloys are approximately 40% lighter than steel and about 36% 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.

In 2004 it was determined by FEA modeling, that cast Ti-6Al-4V can replace cast iron in the engine block and might be able to replace cast iron in the engine head at the standard 305 hp rating if something can be done to lower the temperature in valve bridge regions of the head.
In 2005 the use of a high thermal conductivity material as an insert in the valve bridge areas will be explored by FEA modeling. Also, the modeling will show whether by using Ti in place of cast iron, the engine can be up-rated to 450 hp without changing the basic design of the engine.

Task 2: Magnesium is lighter than both Al and Ti. If Mg can be used to replace cast iron in a heavy-duty diesel engine head and block, the engine's weight can be reduced by up to 35%. This task will determine by FEA modeling, whether a high performance Mg casting alloy can replace cast iron at the standard hp engine rating in a head and/or block.

Task 3: Aluminum alloys are the standard materials for heavy-duty diesel engine turbocharger compressor wheels. The wheels are normally cast using a plaster mold. This process, although acceptable produces a casting with small amounts of porosity. This porosity affects the high-cycle fatigue life of the castings. Semi-solid casting is one way to produce a casting with nearly zero porosity. The traditional semi-solid casting process (Thixomolding) is expensive and requires very high pressures to fill the mold. This is not amenable to compressor wheel casting. A new casting method, Sub-Liquidus Casting (SLC), is a much less expensive method of producing semi-solid castings. Also, it requires one third the pressure to fill the mold as the traditional Thixomolding process. This project will determine the mechanical properties of castings made by the SLC process and compare the data to that produced by permanent mold casting. After that, the process will be evaluated to determine if it is amenable to making composite materials.

Keywords: Titanium Alloys, Ti Alloys in Diesel Engines

49. MECHANICAL BEHAVIOR OF CERAMIC MATERIALS FOR HEAVY DUTY DIESEL ENGINES
    $275,000
    DOE Contact: James J. 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 models and quantifies "quasi-plasticity and fracture thresholds" in ceramics and examines the competing mechanisms that dictate when and how quasi-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., piezoRaman spectroscopy, scanning acoustic microscopy, optical coherent tomography) will be used that will supplement the study and interpretation of the quasi-plastic and fracture thresholds. Specific ceramics are chosen for examination because 1) of their good potential to exhibit quasi-plasticity, or 2) their apparent quasi-plasticity is already established and therefore serves as appropriate model and reference materials for the study of plasticity fundamentals, or 3) quasi-plasticity may be potentially induced, promoted, and exploited through the concurrent application of mechanical loading (e.g., confinement) 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 quasi plasticity and fracture behaviors are relevant for comparison. The thorough understanding of the competition of fracture and quasi-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

50. POWDER PROCESSING OF NANOSTRUCTURED ALLOYS PRODUCED BY MACHINING
$110,000
DOE Contact: James J. Eberhardt, (202) 586-9837
ORNL Contact: D. R. Johnson, (865) 576-6832
Purdue Contact: Srinivasan Chandrasekar, (765)49-43623

This program seeks to capitalize on the recent discovery of a low-cost means of producing nanostructured materials in essentially any metal or alloy by normal machining. Of primary importance is identifying and quantifying the trade-offs between thermal processing and coarsening effects on the intrinsic structure and properties of these new materials. FY2005 activities toward theses goals will focus on four areas as follows: 1) *In-situ* x-ray diffraction line broadening studies will be initiated in collaboration with HTML to provide rapid assessment of changes in grain size with time and temperature. Complimentary characterization via TEM will also be conducted, both at Purdue and in collaboration at HTML; 2) Small-scale powder extrusion and powder rolling studies will be initiated at Purdue, initially using Al 6061-T6 chip based powders.; 3) A study will be conducted to establish the feasibility of rapid infiltration processing using Al-356 to infiltrate tool steel chip preforms under pressure. Use of the die casting facilities at HTML is also anticipated; and 4) Polymer bonding of nanochip aluminum alloy powders will be investigated using epoxies. The degree of metal-polymer adhesion and composite mechanical integrity will be evaluated by tensile testing and fractography.

Keywords: Nanostructured Materials, Metal Nanoparticles

51. DEFORMATION PROCESSES FOR THE NEXT GENERATION CERAMICS
$95,000
DOE Contact: James J. 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, many 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, 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% 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 (1) required for the high permanent strains (>50%) to be able to hot form them and (2) to attain plastic strains of 1 to 5% to enhance their fracture resistance and reliability at lower temperatures. The hot forming study will extend the findings of super plastic (strains ≥100%) 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. Baseline studies are currently establishing the temperature dependence of the deformation response of zirconia ceramics with grains sizes >100 nm but <500 nm. These studies will be extended to <100 nm grain sized ceramics supplied by Subtask 4.24 (Synthesis of Nanocrystalline Ceramics). This will include 1) nanostructured ceramics to explore for the softening effects observed nanocrystalline metals, and 2) the application of external factors (e.g., electric fields) that have been shown to enhance deformation processes in ceramics who’s bonding have some ionic character.

Keywords: Nanostuctured Ceramics, Nanocrystalline Ceramics

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

Third Wave Systems will provide following simulation capabilities to ORNL as part of participation in the project: Drilling of titanium and verification of the 3D machining model for the drilling process. The drilling process from 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. This will include parametric drill design for use in the simulation models and solid model STL import capability. Recommendations for process improvements in material removal rate for deep hole drilling process without compromising the part quality. Baselines will be established in agreement with ORNL.

The verification or the validation process involved for the above will be done with the data provided by ORNL and or University of Michigan. This may be in terms of forces, chip formation, temperature and residual stress.

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

53. WALKER PROCESS FOR STRESS RELIEF
$5,000
DOE Contact: James J. 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

54. SYNTHESIS OF NANOCRYSTALLINE CERAMICS
$45,000
DOE Contact: James J. 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 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% 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.

The focus of research during the past quarter has been the washing and dispersion of high-yield nano-zirconia suspensions. The procedure developed by Kimel *et al.* called for displacement washing (6-7 supernatant replacements) of zirconia suspensions using 10^{-3} M oxalic acid adjusted to pH 9-10 with 2.43 M tetraethylammonium hydroxide (TEAOH). This same procedure was applied to zirconia suspensions of higher yield without successful dispersion. After as many as 10 washes, micron-scale agglomerates persisted within the suspension. It was evident that the concentration of oxalic acid in the wash solution was not sufficient for the dispersion of the higher yield of zirconia. Oxalic acid concentration was increased to 10^{-2} M, which resulted in more well-disperse suspensions.

The next research goal is the removal of water from filter-pressed zirconia pellets while avoiding cracking within the body. It has been proposed that water removal may be accomplished by pushing a non-aqueous solvent through the filter-pressed body immediately after pressing. Several solvents have been suggested: ethanol, methylethyl ketone (MEK), isopropanol, and acetone. Preliminary experiments are in progress.

Keywords: Nanocrystalline Ceramics, Nanocrystalline Oxide Ceramics

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

Mechanical and physical characterization of two TiAl alloys will be completed and compiled in a database. The second iteration of aerodynamic and structural design of a TiAl turbine wheel will be completed, increasing its aerodynamic performance and reducing its operating stresses. Prototype TiAl shafted wheels will be produced and assembled in turbocharger test units. Performance will be evaluated with gas stand and engine testing and compared to the performance of turbochargers built with standard Inconel turbine wheels. Results from these tests will be used to define final modifications and produce turbochargers for field engine testing.

Keywords: Turbocharger, Lightweight Titanium Alloys

56. SURFACE MODIFICATION OF ENGINEERING MATERIALS FOR HEAVY VEHICLE APPLICATIONS
$200,000
DOE Contact: James J. 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

57. IEA IMPLEMENTING AGREEMENT FOR A PROGRAMME OF RESEARCH AND DEVELOPMENT ON ADVANCED MATERIALS FOR TRANSPORTATION APPLICATIONS
    $190,000
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832

The current mission of the implementing agreement on advanced materials for transportation (IA-AMT) is to investigate promising new technologies for evaluating and ultimately improving the performance of materials for transportation systems. The primary motivation for this activity is the fact that new material technologies are required to increase efficiency and reduce harmful emissions in these systems. Examples of these technologies include: 1) light weighting to improve fuel efficiency, 2) surface engineering to improve the resistance to wear and contact damage, 3) development of durable coating systems for thermal, wear, and environmental management, and 4) development of revolutionary materials (structural ceramics and ceramic matrix composites) for operation at much higher temperatures and pressures. The research activities within the IA-AMT focus specifically on: 1) the identification of promising new technologies for improving materials performance and 2) the development of specialized characterization techniques for validating the applicability of this technology to improve material properties while maintaining acceptable life-cycle costs.

At present the contracting parties for the IA-AMT are:

Belgium -The Flemish Institute for Technological Research VITO (Belgium)

Germany - Bundesanstalt für Materialforschung und–prüfung (BAM)

Japan -The New Energy and Industrial Technology Development Organisation (NEDO)

Sweden -The Swedish National Energy Administration (STEM)

United Kingdom - Department of Trade and Industry

United States -The U.S. Department of Energy

Keywords: IEA, Materials Characterization

58. TESTING STANDARDS
    $75,000
    DOE Contact: James J. Eberhardt, (202) 586-9837
    ORNL Contact: D. R. Johnson, (865) 576-6832
    NIST Contact: George Quinn, (301) 975-5765

This project develops mechanical test methods and formal standards for new materials that may be used in diesel engines and other Heavy Vehicle Propulsion Materials applications. The goal is to expedite the utilization of new materials in engines. Prestandardization research will be done to develop new test methods or refine existing methods. Mature methods will then be standardized by organizations such as the American Society for Testing and Materials or the International Organization for Standards, so that designers and engineers can test and evaluate new materials effectively and generate sound databases. Standard Test Methods and Reference Materials will aid the transition of new materials from the laboratory to engineering applications. Engineers will have more confidence using the new materials if the data are generated by formal standard methods. Past work has succeeded in developing test methods for rectangular shaped specimens, but this work needs to be expanded to encompass round shapes such as valves, fuel injector pins, and rollers that are commonly engine parts. New strength test methods for cylindrical shaped brittle materials shall be standardized. This will include the flexural strength of cylindrical rod specimens and split–segmented cylinder shapes. The diametral compression strength test will also be standardized.

Keywords: Standards, ASTM, Fracture Toughness, Flexural Strength

59. IEA - ROLLING CONTACT FATIGUE
    $65,000
    DOE Contact: James J. 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 (HSWR) MATERIALS

60. APPLICATION OF INNOVATIVE MATERIALS
$1,116,000
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: Caterpillar, Freightliner, PACCAR, Volvo, NCC, NIST

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, novel carbon-based materials for thermal management, advanced polymer composites, as well as innovative application of hybrid materials, e.g. lightweight metals with polymer composites.

Keywords: Materials, Carbon-Based Materials, Thermal Management, Polymer Composites

61. LIGHTWEIGHT VEHICLE STRUCTURES
$2,046,000
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, NCC, Heil Trailer, International Truck and Engine, PACCAR, Volvo Trucks, Mack 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, magnesium, 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%. 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

62. MATERIALS PROCESSING DEVELOPMENT
$262,000
DOE Contact: James Eberhardt, (202) 586-9837
ORNL Contact: Phil Sklad, (865) 574-5069
Laboratory Partners: Oak Ridge National Laboratory, Argonne National Laboratory
Industry Partners: Freightliner, PACCAR, Eck Industries

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 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, Truck, Automotive, Aluminum Castings, Oxidation, Polymer Composites, Carbon Fiber

63. MATERIALS DEVELOPMENT
$2,163,000
DOE Contact: James Eberhardt, (202) 586-9837
ORNL Contact: Phil Sklad, (865) 574-5069
Laboratory Partners: Oak Ridge National Laboratory, Pacific Northwest National Laboratory
Industrial Partners: Caterpillar, GS Engineering, Oshkosh Truck, Boler
University Partners: Brown University, University of Tennessee, University of Virginia, Ohio State University

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 developing low-cost powder titanium materials for heavy vehicle applications, non-conventional materials for structural applications, such as metal matrix composites and polymer composites, and innovative materials for brake applications.

Keywords: Simulation Tools, Steel, Titanium, Microstructure, Magnesium, Metal Matrix Composites, Wear, Brakes

64. ENABLING TECHNOLOGIES
$2,105,000
DOE Contact: James Eberhardt, (202) 586-9837
ORNL Contact: Phil Sklad, (865) 574-5069
Laboratory Partners: Argonne National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Los Alamos National Laboratory, Idaho National Laboratory,
University Partners: Tennessee Technological University, University of Tennessee, South Dakota School of Mines

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, and innovative approaches to manufacturing.

Keywords: Joining, Surface Modification, Corrosion, Friction, Equal Channel Angular Extrusion, Ultrasonic Joining, Friction Stir Joining and Processing, Lost Foam Casting, Tooling

HIGH TEMPERATURE MATERIALS LABORATORY

65. 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

66. NEW HIGH-RATE ELECTRODE FOR LITHIUM-ION BATTERIES
$50,000
DOE Contact: Dave Howell, (202) 586-3148
ANL Contact: Gary Henriksen, (630) 252-4591
ANL Principal Investigator: Khalil Amine, (630) 252-3838

Argonne National Laboratory is developing a new anode material for the next generation of high power lithium-ion batteries. The electrodes are based on the inherently high rate lithium manganese oxide spinel cathode material, and the, to date, low rate lithium titanate material. The spinel material has historically suffered from poor capacity fade, however this issue is significantly mitigated by the titanate anode. The latter has been formulated in a new, nanocomposite fashion which provides very high rates, well matched to the spinel material. In addition, both materials are made of relatively low-cost components and to date have shown very promising abuse characteristics. Thus, the new electrode materials could significantly enhance the power density, affordability, and abuse tolerance of lithium-ion batteries for use in hybrid electric vehicles (HEVs). Efforts are underway to scale up the manufacture of the titanate anode material.

Keywords: Li-Ion Battery Anode Materials, High Rate Li-Ion Batteries, Nano Materials

67. BINDER- AND CARBON-FREE OXIDE ELECTRODES FOR DIAGNOSTIC STUDIES
    $100,000
    DOE Contact: Dave Howell, (202) 586-3148
    ANL Contact: Gary Henriksen, (630) 252-4591
    ANL Principal Investigator: Daniel Abraham, (630) 252-4332

Argonne National Laboratory is developing new binder- and carbon- free oxide electrodes to facilitate diagnostic studies related to the formation cycling, low-temperature performance, and aging of lithium-ion cells. Electrodes containing layered-oxide and spinel-oxide materials may be prepared by this technique to study oxide/electrolyte interface reactions during cell cycling and to examine kinetic properties of lithium transport in the oxide structure. Currently $Li_{1+x}Ni_{1/3}Mn_{1/3}Co_{1/3}O_2$ electrodes are being studied, in collaboration with Lawrence Berkeley and Brookhaven National Laboratories, to identify the oxide's role in cell capacity fade and impedance rise.

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

68. NEW HIGH ENERGY ANODES FOR IMPROVED Li ION BATTERIES
    $75,000
    DOE Contact: Dave Howell, (202) 586-3148
    LBNL Contact: Venkat Srinivasan, (510) 495-2679
    SUNY Principal Investigator: Stanley Whittingham, (607) 777-4623

New nano-sized alloys are being developed as possible "next generation" high energy anode materials. Recently, a commercial nanometer-sized tin-cobalt amorphous anode material has been investigated. The material was found to be essentially amorphous, with grain sizes on the order of 10 nm. The electrochemical behavior of this amorphous tin-cobalt anode exhibits none of the two-phase behavior typical of crystalline tin (which suffers rapid capacity fade); rather they show behavior typical of a single-phase reaction. After the ~200mAh/g first cycle loss, the capacity stabilizes near 400mAh/g and is retained much better than for the crystalline tin samples. The new nano-sized material loses approximately 15% of its capacity over the first 40 full charge/discharge cycles whereas the crystalline tin material loses approximately 66% in the first 20 charge/discharge cycles.

Keywords: Li-Ion Battery Anode Materials, High Capacity Li-Ion Batteries, Nanomaterials

69. STABILIZATION OF HIGH-RATE Mn SPINEL CATHODE MATERIALS
    $100,000
    DOE Contact: Dave Howell, (202) 586-3148
    LBNL Contact: Venkat Srinivasan, (510) 495-2679
    U TEXAS Principal Investigator: Arumugam Manthiram, (512) 471-1791

The University of Texas at Austin is developing fluorine substituted manganese spinel oxides that exhibit superior electrochemical performance compared to the oxide analogs. To identify the origin of the enhancement in capacity retention, this group has monitored the evolution of the cubic to cubic phase transition and the two-phase region that occurs during the charge discharge process and the amount of manganese dissolution. It is found that certain cationic substitutions and fluorine substitution lower the lattice parameter difference Δa between the two cubic phases, and the capacity fade at elevated temperatures (60ºC) decreases with decreasing Δa. Also, the cationic and fluorine substitutions decrease the amount of Mn dissolution and the capacity fade decreases with decreasing Mn dissolution. This work is leading the effort towards stabilizing this high rate, abuse tolerant, and low cost material.

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

70. UNDERSTANDING TRANSPORT IN LITHIUM IRON PHOSPHATE
    $250,000
    DOE Contact: Dave Howell, (202) 586-3148
    LBNL Contact: Venkat Srinivasan, (510) 495-2679
    LBNL Principal Investigator: Venkat Srinivasan, (510) 495-2679

This investigation is working to understand and improve the inherent rate capability of the low-cost and abuse tolerant lithium iron phosphate material. Previously, they have predicted a path dependent impedance in the $LiFePO_4$ system, whereby the high-rate electrochemical behavior at a particular State of Charge (SOC) depends on the history by which the electrode was brought to that SOC. For example, the calculated area specific impedance (ASI) during charge is either 50 W-cm^2 or 70 W -cm^2, depending on the cycling history. The lower value occurs when the electrode is brought to 50% from the fully-charged state and the higher value when the electrode is brought to 50% from the fully-discharged state. Further, for the same cycling history, the ASI is different for discharge than for the regen pulse. More interestingly, while the value is higher for the regen pulse compared to the discharge pulse when the electrode is brought to 50% SOC from the fully-discharged state, the value is lower for the regen when the electrode is brought to 50% SOC from the fully-charged state.

The implication of this study is that predicting the power capability of the $LiFePO_4$ system is not straightforward and a clear understanding of the cycling history is necessary. In addition, reporting values of ASI in this material may not provide all the needed information; the cycling conditions under which the value was obtained are needed.

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

GEOTHERMAL TECHNOLOGIES PROGRAM

	FY2005
GEOTHERMAL TECHNOLOGIES PROGRAM TOTAL	$335,000
GEOTHERMAL MATERIALS	$335,000
Heat Exchangers and Condenser Coating Materials	130,000
Advanced Coating Materials	75,000
Acid Resistant Cements	130,000

GEOTHERMAL TECHNOLOGIES PROGRAM

GEOTHERMAL MATERIALS

PROGRAM GOALS

The ultimate goal of the program is to develop advanced cost-effective high-temperature coatings and cementitious materials that can solve corrosion, erosion, and scale deposit problems of metallic components in geothermal power plants and geothermal wells at low pH and brine temperatures up to 350˚C. Success of the program 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 of geothermal energy.
The DOE contact is Raymond LaSala, (202) 586-4198

MATERIALS PREPARATION, SYNTHESIS, PROCESSING, CHARACTERIZATION OR TESTING

71. HEAT EXCHANGER AND CONDENSER COATING MATERIALS
$130,000
DOE Contact: Raymond LaSala, (202) 586-4198
BNL Contact: Toshifumi Sugama, (631) 344-4029

The objectives of this program are to identify thermally conductive lining and coating materials suitable for mitigating corrosion and the deposition of scales on carbon steel heat exchanger (HX) tubes and aluminum-finned steel tubing condensers. It also aims to develop lining and coating technologies that confer the maximum corrosion- and fouling-preventing performance of the candidate material systems, and can be scaled up. The approach to identifying them includes field exposure tests of lined 20-ft.- and 40-ft.-long HX tubes using a BNL-developed state-of-the-art lining apparatus, and also of coated condensers at the Mammoth and Puna geothermal power plant sites in collaboration with the NREL and the private sectors; post-test analyses of these materials are undertaken after the field validation tests. The results from latter provide information on the improvements in the material's formulation and placement technology.

Regarding the HX tube's liners, considerable attention is paid to evaluating the ability of the thermally conductive, self-healing polyphenylenesulfide (PPS) composite lining system being developed by BNL to protect HX tubes against corrosion and to minimize irremovable scale deposits 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. Although a field exposure test at Puna was for only four weeks, the results form post-test analyses demonstrated that this liner withstood a 200˚C brine temperature and displayed a high potential for use as a high-temperature anti-corrosion and –fouling liner. 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. 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.

Regarding the condenser's coatings, with the increased demand for selling electricity in geothermal binary plants during the most valuable summer season, one very important issue is the impairment of the efficiency of the air-cooled condensers, thereby causing ~ 30 % reduction in the plant's net monthly energy delivery compared with that in the winter. A simple method to deal with this problem is to spray directly inexpensive relatively clean cooled geothermal brine over the surfaces of the aluminum-finned steel tubing condenser. As expected, such sprayed condensers attained an output of the same generating capacity for electricity as under wintertime conditions. Although this method is very attractive, a concern raised about spraying the brine is the likelihood of corroding the condenser's components, aluminum fins and carbon steel tubes, as well as depositing geothermal brine-induced mineral scales on them. To deal with this problem, our work is devoted to optimizing the formulation of the BNL-developed water-based aminopropylsilane triol (APST) precursor solution suitable for a simple dip-withdrawing coating technology. The precursor solution is compatible with both metals. The precursor-wetted condensers, then is placed in air at 150˚C to convert the precursor into the solid polyaminopropylsiloxane (PAPS), a member of a family of organometallic polymers (OMP). The PAPS films are deposited on the condensers for a field validation test that is performed using the NREL-designed brine sprayer apparatus, installed in the maintenance building at the Mammoth power plant. The success will offer the following potential benefits: An increased efficiency in the summer season, and an increased operational flexibility and control schemes that can maximize power production during periods of high power demand, thereby increasing revenue.

Keywords: Heat Exchanger, Aluminum-Finned Condenser, Corrosion, Scale Deposits, Carbon Steel, Liners, Coatings

72. ADVANCED COATING MATERIALS
$75,000
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 task of this program is divided into four subtasks: The first subtask is to formulate 300˚C-stable polyphenylenesulfide (PPS) and polyetheretherketone (PEEK) thermoplastic coatings using nanocomposite technologies for wellhead and heat exchanger components; the second is to develop new types of nanoscale rare earth metal oxide-doped organometallic polymer (OMP) coatings using BNL's technology for synthesizing self-assembly nanocomposites for condensers; the third is to establish the surface-processing technology that will confer low friction and low surface free energy to the coating for steam separators; and, the fourth subtask is to identify low temperature-curable thermosetting polymer-based coatings possessing a hydrothermal stability of >200˚C for the exchanger tube/sheet and pipe/pipe joint areas after rolling-in or welding. Its success would provide information on new material synthesis, processing technologies, and the specific characteristics of materials, as well as on eventually scaling up coating technologies necessary to adequately protect inexpensive carbon steel-based plant's components in corrosive geothermal environments. Thus, once the developed materials are applied to plant's components, they will improve the power plant's economic factors, including a considerable reduction of the needed capital investment, and a decrease in the costs of operations and maintenance through optimized maintenance schedules.

Keywords: Coatings, Corrosion, Polymer Nanocomposite, Organometallic Polymer, Teflon, Plant Components, Tube/Sheet Joints

73. ACID RESISTANT CEMENTS
$130,000
DOE Contact: Raymond LaSala, (202) 586-4198
BNL Contact: Toshifumi Sugama, (631) 344-4029

The program has the following three objectives: The first is to develop a cost-effective alkali-activated slag cementitious material containing a large amount of anti-acid zeolite phases as an advanced acid-resistant cement; the second is to modify a low-density air-foamed calcium aluminate phosphate (CaP) cement slurry with waterborne acrylic-based polymer additives in improving the corrosion-preventing performance of foamed CaP cement; and third aim is to conduct a hot-cold cycling fatigue test to evaluate the durability of bonds at interfaces between carbon fiber-reinforced tough cements and casing pipes. The primary goal of the first objective is to formulate commercial 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, and yet the formulated cements would cost less than ordinary Portland cement (4.4 ¢/lb). The goal of second objective is to design a 200°C-stable polyacrylic-modified CaP foam cement with a slurry density of <1.22 g/cc, and also the hardened cement is required to reduce considerably the corrosion rate of carbon steel casing, <2.0 milli-inch per year, and minimize NaCl conductivity through the cement layer, pore resistance >400 ohm-cm^2. In the third objective, the one critical issue of the casing's corrosion concerned the generation of fissures in the cement adhering to the casing caused by an irregularly pulsating superheated fluid or steam. Thus, the goal of this objective is to assess the bond durability of fiber-reinforced tough cement composites adhering to casing's surface in a superheat-cold cycling fatigue test (ranging from 25-250˚C) of the composite-sheathed casings. The integration of all the information obtained in these objectives will provide advanced cement technologies necessary for successful wellbore completions in a corrosive geothermal environment.

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

HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM

	FY 2005
HYDROGEN, FUEL CELLS AND INFRASTRUCTURE TECHNOLOGIES PROGRAM GRAND TOTAL	$20,368,055
FUEL CELL MATERIALS	$625,000
Microstructural Characterization of PEM Fuel Cells	300,000
Cost-Effective Metallic Bipolar Plates Through Innovative Control of Surface Chemistry	325,000
HYDROGEN PRODUCTION MATERIALS PROGRAM	$1,950,000
Photoelectrochemical Systems for H_2 Production	800,000
Photoelectrochemical Hydrogen Production Program	575,000
Discovery of Photocatalysts for Hydrogen Production	250,000
Photoelectrochemical Hydrogen Production Using New Combinatorial Chemistry Derived Materials	200,000
Solar Water Splitting: Photocatalyst Materials Discovery and Systems Development	25,000
Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen	100,000
HYDROGEN STORAGE MATERIALS PROGRAM	$17,793,055
CHEMICAL HYDROGEN STORAGE	$5,985,000
Chemical Hydrogen Storage Center of Excellence	3,901,000
Carbon-Based Sorbent Systems for Containment of H2/ H2 Carriers	812,000
Low-Cost Off-Board Regeneration of Sodium Borohydride	716,000
Chemical Hydride Slurry	356,000
Development of Regenerable, High-Capacity Boron Nitrogen Hydrides	200,000
METAL HYDRIDE HYDROGEN STORAGE	$6,250,000
Metal Hydride Center of Excellence	5,000,000
Materials Discovery	562,055
Complex Metal Hydrides Using Molecular Modeling and Combinatorial Methods	550,000
Effects and Mechanisms of Mechanical Activation on Hydrogen Sorption/Desorption of Nanoscale Lithium Nitrides	138,000
CARBON AND HIGH SURFACE AREA SORBENTS	$4,243,000
Carbon Materials Center of Excellence	3,803,000
Carbide-Derived Carbons with Tunable Optimized Porosity	300,000
Nanostructured Activated Carbon	80,000
Electron-Charged Graphite	60,000
NEW MATERIALS AND CONCEPTS	$1,315,000
Sub-Nanostructured Non-Transition Metal Complex Grids	190,000
Hydrogen Storage in Metal-Organic Framework Structures	112,000
Synergistic Approach to Development of New Classes of Hydrogen Storage Materials	500,000
Novel Metal Perhydrides	50,000
Hydrogen Storage Materials with Unsaturated Metal Binding Sites	113,000
Hollow Glass Microspheres for Hydrogen Storage	100,000
Hydrogen Storage in Novel Molecular Materials	200,000
Hydrogen Storage in Novel Organic Clathrates	50,000

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 Patrick Davis, (202) 586-8061.

Fuel cells are one of the key enabling technologies for a future hydrogen economy. They 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 in the near-term on fuel cell systems running on natural gas or propane and recognizes the longer term potential for systems running on renewable fuels. The DOE/EERE contact for fuel cells is Valri Lightner, (202) 586-0937.

FUEL CELL MATERIALS PROGRAM

74. MICROSTRUCTURAL CHARACTERIZATION OF PEM FUEL CELLS
$300,000
ORNL Contact: T. R. Armstrong, (865) 574-7996
DOE Contact: N. L. Garland, (202) 586-5673

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 electrocatalysts are being quantified 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). Extensive catalyst particle coarsening (loss of surface area) and Pt migration into the Nafion® membrane were observed and explained the performance decay observed (loss of 54 mV) during 1,000 h of cell operation.

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: PEM, Fuel Cells, Microstructure, Characterization

75. COST-EFFECTIVE METALLIC BIPOLAR PLATES THROUGH INNOVATIVE CONTROL OF SURFACE CHEMISTRY
$325,000
ORNL Contact: T. R. Armstrong, (865) 574-7996
DOE Contact: N. L. Garland, (202) 586-5673

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 has 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 5-10x less than the Ni-Cr base alloys studied/developed under this effort. In addition, this is the first time such a surface has been successfully formed on a Fe-Cr base alloy. (This surface is more robust and corrosion-resistant 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 warping was observed, and although some technical challenges exist, no “show stopper” phenomena were observed in this first attempt.

Keywords: Bipolar Plates, Testing, Alloys

HYDROGEN PRODUCTION MATERIALS PROGRAM

PHOTOELECTROCHEMICAL PRODUCTION OF HYDROGEN

76. PHOTOELECTROCHEMICAL SYSTEMS FOR H_2 PRODUCTION
$800,000
National Renewable Energy Laboratory Contact: John A. Turner
DOE Contact: Roxanne Garland, (202) 586-7260

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 2005, NREL's study of PEC direct conversion systems involved two areas of materials research focusing on possible high-efficiency materials with greater corrosion resistance and low-cost thin-film materials for application as protective coatings against corrosion, and as possible water splitting systems.

Keywords: Photoelectrochemical, Hydrogen Production

77. PHOTOELECTROCHEMICAL HYDROGEN PRODUCTION PROGRAM
    $575,000
    Hawaii Natural Energy Institute, University of Hawaii at Manoa Contact: Eric L. Miller
    DOE Contact: Roxanne Garland, (202) 586-7260

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, establishment of industry and university partners with thin-film materials expertise, and fabrication and evaluation of photoelectrode test devices.

Keywords: Photoelectrochemical, Hydrogen Production

78. DISCOVERY OF PHOTOCATALYSTS FOR HYDROGEN PRODUCTION
    $250,000
    SRI International Contact: D. Brent MacQueen
    DOE Contact: Roxanne Garland, (202) 586-7260

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, SRI has designed and built a 25-cell module to analyze the photolysis products generated upon illumination of samples with a simulated solar spectrum. The approach of this project is to take advantage of the high surface area of nanoparticles in increase the efficiency of TiO_2 and TiO_2-based materials. FY2005 will be the last year of DOE funding for this project.

Keywords: Photocatalyst, Hydrogen Production

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

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 (e.g., GaAs, InP, etc.) have generally demonstrated greater efficiency, cost and/or natural abundance could be problematic on a large scale; thus, combinatorial techniques are applied 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 ZnO, Fe_2O_3, and Cu_2O_3 hosts, investigating libraries of variable composition and morphology. They have also developed a pulsed-electrodeposition scheme for depositing nanoparticulate pure metals (Pt, Au, Pd), alloys (Pt-Au, Pt-Ru), and metal oxides (WO_3) which has been incorporated into their automated synthesis and screening systems. In addition, they have developed and automated spray pyrolysis deposition system for synthesis of Fe_2O_3 and ZnO libraries.

Keywords: Photoelectrochemical, Hydrogen Production, Combinatorial Chemistry

80. SOLAR WATER SPLITTING: PHOTOCATALYST MATERIALS DISCOVERY AND SYSTEMS DEVELOPMENT
$25,000
GE Global Research Contact: Thomas F. McNulty
DOE Contact: Roxanne Garland, (202) 586-7260

This project, when significantly funded, will have a two-pronged approach is envisaged, where studies of photoelectrochemical materials occur simultaneously with studies of electron and hole transfer catalysts. The principal focus of this work is to develop photoelectrochemical materials with the durability of oxide materials and the band gap of the non-oxides. Doping of oxide materials on the anion site with elements such as carbon and nitrogen have been performed for photocatalysts such as TiO2. Evidence shows that this can indeed increase the photosensitivity of the system. This work has not been performed in a systematic fashion on materials not requiring an external bias.

Keywords: Photocatalyst, Photoelectrochemical, Solar Water Splitting

81. CRITICAL RESEARCH FOR COST-EFFECTIVE PHOTOELECTROCHEMICAL PRODUCTION OF HYDROGEN
$100,000
Midwest Optoelectronics Contact: Liwei Xu
DOE Contact: Roxanne Garland, (202) 586-7260

This project is developing two aspects toward efficient and durable photoelectrodes for immersion-type photoelectrochemical cells, In the first approach, triple-junction tf-Si based solar cells are used to generate the voltage bias and a transparent, conduction and corrosion resistant (TCCR) coating is deposited on top to protect the semiconductor layer from corrosion while forming an ohmic contact with the electrolyte. The second approach is a hybrid structure in which two tf-Si based junctions provide a bias and a third junction is a rectifying junction between a photo-active semiconductor and the electrolyte.

Keywords: Photoelectrochemical, Hydrogen Production

HYDROGEN STORAGE MATERIALS PROGRAM

CHEMICAL HYDROGEN STORAGE

82. CHEMICAL HYDROGEN STORAGE CENTER OF EXCELLENCE
$3,901,000
DOE Contact: G. Ordaz, (202) 586-8350
Center Coordinator: Los Alamos National Laboratory, W. Tumas
Partners: Intematix Corporation, Xiao-Dong Xiang
Millennium Cell Inc., Ying Wu
Northern Arizona University, Clinton F. Lane
Pacific Northwest National Laboratory, Christopher L. Aardahl
Pennsylvania State University, Digby D. Macdonald
Rohm and Haas Company, Suzanne W. Linehan
US Borax, David Schubert (Does not get funding from DOE)
University of Alabama, David A. Dixon
University of California, Davis, Philip P. Power
University of California, Los Angeles, M. Frederick Hawthorne
University of Pennsylvania, Larry G. Sneddon
University of Washington, Karen I. Goldberg

The purpose of the Center is to conduct a coordinated approach to identify, research, and develop advanced on-board chemical hydrogen storage systems to meet DOE 2010 storage system targets with the potential to meet to 2015 targets. Chemical hydrogen storage involves storing hydrogen in and releasing hydrogen from covalent chemical bonds in molecules and materials. Researchers in the Center are advancing a number of integrated projects involving the development of materials, catalysts, catalytic processes, and new concepts for hydrogen release and regeneration of spent material, as well as the development of engineering feasibility of the processes. Key elements in the Center include computation and modeling; the design, synthesis, and testing of structures and compositions to control the thermochemistry and kinetics of hydrogen release and spent fuel regeneration; and development and assessment of engineering concepts and systems for hydrogen release and regeneration. Engineering studies in the Center will include development, assessment, modeling and testing ranging from process identification through optimization of hydrogen release and regeneration reaction conditions, including catalyst performance and lifetime, and mass transfer to the construction and testing of a prototype for hydrogen release and testing of a process for spent storage material regeneration.

A number of significant preliminary accomplishments have been made. The Center has made significant strides in utilizing high-level quantum chemical calculations to calculate thermodynamics of reactions and key reaction intermediates, which has helped guide discovery and mechanistic experimental efforts. Catalysts and processes that enable hydrogen generation from ammonia-borane (storage capacity of 19.6 weight %), including non-metal and transition metal homogeneous catalysts, nanoparticle heterogeneous catalysts, and inclusion in inorganic scaffolds have been discovered. Regeneration concepts for ammonia-borane are also being developed. Catalysts have also been discovered for polyhedral borane hydrolysis. Extended literature search and some laboratory experiments have been conducted to better understand the possibility for efficient borate reduction. New classes of reactions involving heteroatom organic compounds and coupled reactions for hydrogen release have also been demonstrated. In addition, the center has also developed on-board reactor engineering concepts using lessons learned from a past sodium borohydride on-board reactor prototype.

Keywords: Hydrogen Storage, Chemical Bonding, Catalysts, Borane, Sodium Borohydride

83. CHEMICAL HYDRIDE SLURRY FOR HYDROGEN PRODUCTION AND STORAGE
$356,000
Safe Hydrogen, LLC Contact: A. McClaine
DOE Contact: G. Ordaz, (202) 586-8350

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: Hydride, Slurry, Hydrogen Production, Hydrogen Storage

84. DESIGN AND DEVELOPMENT OF NEW CARBON-BASED SORBENT SYSTEMS FOR AN EFFECTIVE CONTAINMENT OF HYDROGEN
$812,000
Air Products and Chemicals, Inc. (APCI) Contact: A. Cooper
DOE Contact: G. Ordaz, (202) 586-8350

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.

Keywords: Carbon, Sorbent, Hydrogen Containment

85. LOW COST, OFF-BOARD REGENERATION OF SODIUM BOROHYDRIDE
$716,000
Millennium Cell Inc. Contact: Y. Wu, (732) 544-5718
DOE Contact: G. Ordaz, (202) 586-8350

The objective of this project is to develop energy efficient and cost effective new syntheses of sodium borohydride or its precursors. The borohydride molecule can serve as either a hydrogen storage medium or as a precursor to other hydrogen storage species such as boron-nitrogen compounds, or boron–doped metal hydride reversible systems. At the present time, however, it is costly to make sodium borohydride at commodity-scale. Millennium Cell Inc. is working on new or improved electrolysis process for the reduction of borates to borohydrides, and to conduct preliminary engineering studies of the process that they believe are most likely to result in substantial cost savings over present methods.

Millennium Cell Inc. surveyed a number of possible electrolytic pathways and discovered that:

- Borates can be reduced to boron hydrides in a single electrolytic step
- The raw material (sodium) for making borohydride could be produced much more efficiently than previously thought
- Sodium borate spent materials from borohydride hydrolysis could be conveniently reprocessed into starting materials for making borohydride

Knowledge gained from these studies will be applied to updating, modifying, and replacing various steps of the current borohydride synthesis methodology, with an emphasis on process performance improvement, especially in the areas of fuel cost, energy efficiency, and minimizing greenhouse gas emissions. Additional work is needed and continues in order to improve both the overall energy and cost efficiency of the process.

Keywords: Hydrogen Storage, Sodium Borohydride

86. DEVELOPMENT OF REGENERABLE HIGH CAPACITY BORON NITROGEN HYDRIDES AS HYDROGEN STORAGE MATERIAL
$200,000
RTI International Contact: A. Damle
DOE Contact: G. Ordaz, (202) 586-8350

The objective of this project is to develop synthesis and hydrogen extraction processes for nitrogen/boron hydride compounds that will permit exploitation of the high hydrogen content of these materials. The primary compound of interest in this project is aminoborane (NH_3BH_3, ammonia-borane,) a stable white solid at ambient conditions that contain 19.6% of its weight as hydrogen. With a low-pressure on-board storage and an efficient heating system to release hydrogen, aminoborane has a potential to meet DOE's year 2015 specific energy and energy density targets. Amorphous boron nitride (BN) is the desired aminoborane decomposition end-product. If the aminoborane synthesis process could use the BN end-product as the primary starting material, an efficient recycle loop could be set up for converting the BN back into the starting boron-nitrogen hydride.

This project will address two key challenges facing the exploitation of the boron/nitrogen hydrides (aminoborane), as hydrogen storage materials: 1) large-capacity inexpensive aminoborane regeneration process starting from its decomposition by-product, BN for recycle, and 2) a simple, efficient, and controllable system for extracting all of the available hydrogen, realizing the high hydrogen density on a system weight/volume basis

RTI will develop chemical process steps to convert boron nitride to aminoborane, using only hydrogen and commodity chemicals such as ammonia and chlorine, on a laboratory scale. RTI will also study and optimize the process of hydrogen release by thermal decomposition of aminoborane and demonstrate feasibility of regenerating aminoborane decomposition product.

Keywords: Hydrogen Storage, Boron Nitride, Hydrides

HIGH CAPACITY METAL HYDRIDES

87. METAL HYDRIDE CENTER OF EXCELLENCE
$5,000,000
DOE Contact: C. Read, (202) 586-3152
Center Coordinator: Sandia National Laboratory-Livermore Contact: L. Klebanoff and J. Keller
Partners: Brookhaven National Laboratory, Jim Wegrzyn
California Institute of Technology, Channing Ahn
Carnegie Mellon University, David Sholl
General Electric Company, J. C. Zhao
HRL, Greg Olson
Intematix Corporation, Guanghui Zhu
Jet Propulsion Laboratory, Bob Bowman
NIST Center for Neutron Research, Terry Udovic
Oak Ridge National Laboratory, Gilbert Brown
Savannah River National Laboratory, Ted Motyka
Stanford University, Bruce Clemons
University of Hawaii-Manoa, Craig Jensen
University of Illinois, Ian Robertson and Duane Johnson
University of Pittsburgh, Karl Johnson
University of Nevada-Reno, Dhanesh Chandra
University of Utah, Zak Fang

The DOE Metal Hydride Center of Excellence (MHCoE) consists of 8 universities, 3 industrial partners, and 6 national/federal laboratories. SNL is the lead laboratory of the Center to provide leadership for the Center and a management structure to assist and advise the DOE. The goal of the MHCoE is to discover and develop efficient, safe and cost-effective reversible hydrogen storage materials for vehicle applications. To achieve this goal, we have assembled an interdisciplinary team of the best researchers to address each critical component of this technical "Grand Challenge." These components are: 1) materials development and discovery including rapid experimental development efforts, 2) fundamental modeling and science to identify hydrogen-materials interactions and to provide direction for the screening efforts, 3) materials synthesis and improved performance through compositional, structural, catalytic, and nano-synthesis modification, 4) rigorous testing of hydrogen storage and delivery properties to support the fundamental science and to enable a critical and timely evaluation of materials research directions, and finally (5) strong engineering science and process development capabilities to accelerate the transition of the best hydrogen storage materials and systems to a commercial reality.

The Center's project work has just started in FY 2005. Specific progress on current projects and proposed work by the center partners is describe below:

- Identified aluminum hydride (AlH3, theoretical material capacity of 10 wt%) as a promising candidate for meeting DOE's 2010 hydrogen storage goals. Found that the desorption temperature of the as-received α-AlH3, which typically ranged from 175-200°C, could be lowered to 100-150°C when the material was mechanically milled with a LiH dopant (BNL and SNL).
- Refinement and scale-up of synthesis of Si, Mg and MgH2 in nanophase form using a cryo-melting gas condensation technique (CalTech).
- Demonstrated that a high-throughput screening tool based on thermography can screen hydrogen absorption & desorption with a sensitivity down to 0.3 wt% hydrogen (GE).
- LiBH4/Mg(X) appears to represent a class of promising high capacity destabilized systems with partial to complete reversibility demonstrated for X = H, F, and S. However, these systems also display slow kinetics; future work will focus on enhanced reaction rates in nanoscale materials (HRL).
- Validated combinatorial molecular beam epitaxy (MBE) and ion beam sputtering (IBS) systems for synthesizing thin film complex hydrides containing air-sensitive elements, such as Li, Na, Mg (Intematix).
- 5.2 wt% reversible hydrogen storage was achieved through the development of a destabilized Mg-modified Li-imide material (SNL).

Keywords: Hydrogen Storage, Metal Hydrides, Nanoscale Materials, High-Throughput Screening

88. DISCOVERY OF NOVEL COMPLEX METAL HYDRIDES FOR HYDROGEN STORAGE THROUGH MOLECULAR MODELING AND COMBINATORIAL METHODS
$550,000
UOP LLC Contact: D. Lesch
DOE Contact: C. Read, (202) 586-3152

Recently, it has been shown that the complex hydride $NaAlH_4$ can reversibly absorb hydrogen at lower pressures and temperatures than MgH_2 and has a higher gravimetric capacity and lower cost than $LaNi_5H_6$. 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: Hydrogen Storage, Metal Hydrides, Molecular Modeling, Combinatorial Chemistry

89. COMPLEX HYDRIDE COMPOUNDS WITH ENHANCED HYDROGEN STORAGE CAPACITY
$562,055
United Technologies Research Center Contact: D. Moser
DOE Contact: C. Read, (202) 586-3152

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: Hydrogen Storage, Hydrides

90. EFFECTS AND MECHANISMS OF MECHANICAL ACTIVATION ON HYDROGEN SORPTION/ DESORPTION OF NANOSCALE LITHIUM NITRIDES
$138,000
L. Shaw, University of Connecticut, Storrs
DOE Technology Development Manager: C. Read, (202) 586-3152

The University of Connecticut proposes to develop a fundamental understanding of the effects and mechanisms of mechanical activation on hydrogen storage capacity and sorption/desorption processes of nanoscale Li3N. Researchers plan to produce a novel, mechanically activated, nanoscale Li3N-based material that is able to store and release ~10 wt% hydrogen at temperatures below 100˚C. A novel, mechanically activated, nanoscale lithium nitride (Li3N) based material will be researched and developed that has the potential to store hydrogen at high capacities. The project will demonstrate that improvements in the hydrogen sorption/desorption kinetics can be achieved by mechanical activation like ball milling. Many fundamental issues such as how hydrogen reacts with the surface, grain boundaries, and bulk defects of lithium nitrides and hydrides, and what controls the hydrogen storage capacity, both maximum and reversible, in these compounds as a function of mechanical activation will be addressed.

Keywords: Hydrogen Storage, Mechanical Activation, Nanoscale Materials, Lithium Nitride

CARBON AND HIGH SURFACE AREA SORBENTS

91. CARBON MATERIALS CENTER OF EXCELLENCE
$3,803,000
DOE Contact: S. Satyapal/C. Read, (202) 586-3152
Center Coordinator: National Renewable Energy Laboratory Contact: M. Heben and L. Simpson
Partners: Air Products and Chemicals Inc., Alan Cooper
California Institute of Technology, Channing Ahn
Duke University, Jie Liu
Lawrence Livermore National Laboratory (LLNL), Joe Satcher
National Institute of Standards and Technology (NIST), Dan Neumann
Oak Ridge National Laboratory (ORNL), Dave Geohegan
Pennsylvania State University, Peter C. Eklund
Rice University, Richard E. Smalley/James Tour
Rice University, Boris Yakobson and Robert Hauge
University of Michigan, Omar M. Yaghi
University of Michigan, Ralph T. Yang
University of North Carolina (Chapel Hill), Yue Wu
University of Pennsylvania, Alan G. MacDiarmid

The Carbon-based Hydrogen Storage Center of Excellence is developing novel carbon-based and high-surface-area materials and systems for on-board vehicle hydrogen storage. The Center was established during the past year and presently has fourteen active projects at twelve institutions. Center partners are conducting a wide range of research, development and engineering studies on currently available adsorbent materials and developing the design principals and synthetic methods for next-generation materials that will meet the critical DOE 2010 hydrogen storage system targets.

The overall approach of the Center is as follows:

- Design, synthesize and test a number of promising carbon-based and high-surface-area materials for reversible, on-vehicle hydrogen storage.

- Perform detailed experimental and computational investigations to determine the limits of performance of specific materials and extract general mechanistic information.

- Develop an in-depth understanding of the factors affecting adsorbent synthesis and stability to permit the fabrication of materials that are optimized for on-board vehicular hydrogen storage.

- Perform accurate measurements of hydrogen storage capacity as a function of pressure and temperature and characterize material properties and hydrogen storage behaviors.

- Develop methods to reproducibly activate and handle materials to permit scale-up and validation of hydrogen uptake/release.

- Develop and test system configurations that can meet DOE RD&D Plan goals for on-vehicle reversible hydrogen storage.

The FY 2005 Accomplishments of Center include:

- Developed first computational model, based on Kubas-type binding of dihydrogen, for carbon-metal hybrid adsorbents capable of reversibly storing nearly 9 wt% hydrogen at more than 43 kg H_2/m^3 at room temperature and pressure.

- Performed calculations and preliminary experiments to determine hydrogen storage enhancement permitted by incorporating simple metals in sp^2–bonded carbon networks.

- Identified promising wet-chemical and gas-phase synthetic routes to synthesize predicted materials. Commercial samples of polyaniline emeraldine base and nanofibers were chemically treated and tested for hydrogen adsorption/desorption.

- Developed and applied nuclear magnetic resonance (NMR) and neutron scattering spectroscopy techniques to measure hydrogen in candidate materials.

- The locations of hydrogen adsorption sites in a metal organic framework (MOF-5) were determined using neutron powder diffraction.

- Synthesized and characterized boron-doped polymers, single-wall nanotubes (SWNTs), fibers and onions. Assessed H_2/D_2 exchange on adsorbent materials to determine dissociative and non-dissociative hydrogen binding.

- Discovered that hydrogen storage capacities on hotwire chemical vapor deposition generated nano-crystalline graphite could be enhanced by the presence of iron nanoparticles.

- Observed hydrogen adsorbed in MOF-5 by Raman spectroscopy. Reversible physisorption occurred at all pressures employed, including 30 bar. At room temperature, a 10 cm-1 decrease in the hydrogen stretching frequency was measured, indicating a fairly strong interaction.

- Developed a curvature-dependent force field and molecular dynamics model to calculate the optimal distribution of H_2 on SWNTs, the average adsorption energy per H_2, and the electrostatic potential of SWNTs.

- Initiated collaboration in a modeling task to relate system-level performance to component and material capacities, with a focus on volumetric capacities.

- Performed measurements and collected volumetric sorption data from partners for two different carbons to ensure measurement uniformity with partner labs and Southwest Research Institute.

- Synthesized and activated isoreticular metal organic framework (IRMOF) structures with surface areas up to 3080 m^2/gm.

- Prepared series of metal-doped carbon aerogels (MDCAs) containing different metals (i.e., iron, nickel, cobalt) and completed structural characterization.

Keywords: Hydrogen Storage, Sorption, Carbon Materials, Molecular Modeling, Carbon-Metal Hybrids, Carbon Nanotubes, Aerogels

92. ELECTRON-CHARGED GRAPHITE-BASED HYDROGEN STORAGE MATERIAL
$60,000
C. Fan, Gas Technology Institute
DOE Technology Development Manager: C. Read
(202) 586-3152

GTI proposes to develop a new low-cost graphite-based structure with a novel electron charge device that is able to store hydrogen to meet the DOE storage target of 6 wt%. This new concept involves modification of low-cost graphite for hydrogen storage using incorporation of key metals and an electron charge device that will enhance electron charge balance, hydrogen storage capacity, and hydrogen charge/discharge cycle life. After the initial proof-of-feasibility phase, performance optimization will be conducted and production costs and processing will be analyzed for commercial manufacture. New hydrogen storage materials based on low cost natural flake graphite materials will be researched and developed. This concept involves the modification of low cost natural flake graphite for hydrogen storage using the expansion of the graphite layers to allow access for hydrogen adsorption, enhancing hydrogen storage capability of the material.

Keywords: Hydrogen Storage, Graphite

93. NANOSTRUCTURED ACTIVATED CARBON FOR HYDROGEN STORAGE
$80,000
I. Cabasso, State University of New York at Syracuse
DOE Technology Development Manager: C. Read,
(202) 586-3152

SUNY-Syracuse proposes to develop a novel methodology for the preparation of nanostructured activated carbon for hydrogen storage and demonstrate attainment of 6% (by weight) hydrogen storage capacity. They also plan to demonstrate sustainability of attained sorption capacity and design to scale the process to prepare kilogram quantities of the material. They also plan to extend hydrogen sorption capacity to 8% (by weight). Novel nano-structured activated carbons for hydrogen storage will be researched and developed. The novel methodology employs a nanoporous polymeric precursor for the carbon adsorbent preparation. These high surface area materials will significantly increase the hydrogen storage capacity of the activated carbon.

Keywords: Hydrogen Storage, Nanostructured Materials, Carbon

94. CARBIDE-DERIVED CARBONS WITH TUNABLE POROSITY OPTIMIZED FOR HYDROGEN STORAGE
$300,000
University of Pennsylvania Contact: J. Fischer
Drexel University Contact: Y. Gogotsi
DOE Technology Development Manager: C. Read, (202) 586-3152

The University of Pennsylvania and Drexel University propose to develop and demonstrate reversible hydrogen storage in carbide-derived carbons (CDC) with tunable nanoporosity. They plan to determine the optimum pore size for hydrogen storage using experiment and theory, and to design a CDC-based hydrogen storage material that meets the DOE performance targets and is commercially viable. Carbide-derived carbons (CDC) are expected to have a greater hydrogen storage capacity than all of the other carbons studied to date. The reason is that CDC pore size can be precisely tuned to match the appropriate molecular diameter, with a better than 0.5 Å accuracy in the range 5-15 Å, by optimizing the choice of precursor carbide and chlorination temperature. Specific surface area (SSA) of up to 2,000 m2/g and up to 80% open pore volume are readily achievable, and the materials are projected to be very cheap compared to e.g. nanotubes.

Keywords: Hydrogen Storage, Carbon, Carbides, Nanostructured Materials

NEW MATERIALS & CONCEPTS

95. SUB-NANOSTRUCTURED NON-TRANSITION METAL COMPLEX GRIDS FOR HYDROGEN STORAGE
$190,000
Cleveland State University Contact: O. Talu
DOE Technology Development Manager: C. Read, (202) 586-3152

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: Hydrogen Storage, Nanostructured Materials, Metal Grids

96. A SYNERGISTIC APPROACH TO THE DEVELOPMENT OF NEW CLASSES OF HYDROGEN STORAGE MATERIALS
$500,000
J. R. Long, University of California-Berkeley
Partner: Lawrence Berkeley National Laboratory
DOE Technology Development Manager: C. Read, (202) 586-3152

The University of California-Berkeley proposes to develop and demonstrate new types of hydrogen storage materials with at least 6 wt.% materials-based gravimetric capacity and with potential to meet DOE 2010 system-level targets. Materials under consideration include nanoporous polymers, nanoporous coordination solids, destabilized high-density hydrides, nanostructured boron nitride and magnesium and metal alloy nanocrystals. Theoretical work includes first-principles determination of hydrogen binding energies and development of theory on boron nitride-containing nanostructures. A team of scientists will explore new materials with the potential to store hydrogen at high capacities. Nanoporous coordination solids and polymers with exceptionally high surface areas will be included, exploiting a new templating synthesis technique. Boron nitride-containing structures with a high affinity for H2 will also be targeted based on guidance from theoretical work. The effects of size and shape on the hydrogen storage characteristics of magnesium and metal alloy nanocrystals will also be studied.

Keywords: Hydrogen Storage, Nanostructured Materials, Hydrides, Boron Nitride, Alloys

97. HYDROGEN STORAGE IN NOVEL MOLECULAR MATERIALS
$200,000
Carnegie Institution of Washington Contact: V. Struzhkin
DOE Contact: G. Ordaz, (202) 586-8350

Carnegie Institution of Washington is conducting fundamental studies of inorganic H_2 clathrates (H_2O- and CH_4- based). Computer simulation study of binary and ternary systems are conducted to understand structural details and stability. Insights gained from these studies will be applied toward the design and synthesis of hydrogen storage materials that meet the DOE 2010 hydrogen storage targets, especially cost, specific energy, energy density, environmental cleanliness, and safety of hydrogen storage. Clathrates with very high H_2 contents were synthesized in diamond anvil cells at high pressure (P) and low temperature (T); clathrate formation and hydrogen release are spontaneous. The challenge is to extend the P-T stability field to near ambient P and T. Carnegie Institution of Washington is attempting to stabilize the clathrates with additional guest molecules (promoters).

Reversible hydrogen storage with 4% weight capacity has been already demonstrated for THF-H_2O sII clathrate at 270˚K and 12 MPa by H. Lee ET. Al. (Nature 434, p. 743, 2005). Carnegie Institution of Washington has preliminarily demonstrated that addition of THF moves the stability line for H_2-sII clathrate to nearly room temperature at P>50 MPa. The stability line is strongly nonlinear, suggesting that THF-stabilized H_2 clathrate could exist above 250˚K at ambient pressure. The sH clathrate with methylcyclopentane (C_6H_{12}) could be another candidate for H_2 storage, due to even larger cages than in sI and sII clathrates.

Keywords: Hydrogen Storage, Clathrates

98. HYDROGEN STORAGE IN NOVEL ORGANIC CLATHRATES
$50,000
University of Missouri-Columbia Contact: J. Atwood
Partner: B. Peter McGrail, Pacific Northwest National Laboratory
DOE Contact: G. Ordaz, (202) 586-8350

Many hydrogen storage methods have been proposed based on physical adsorption on activated carbons, zeolites, carbon nanotubes and metal-organic frameworks, but each has its technical challenges. University of Missouri-Columbia is utilizing the principles of crystal engineering and molecular self-assembly to develop a new class of organic clathrates that represent a fundamentally new method for high-density storage of hydrogen and to demonstrate DOE's 2010 capacity target of 6 wt% hydrogen storage.

The university will first synthesize clathrates from monomers such as p-cresol, phenol, beta-quinol, Dianin's compound, urea, and thiourea. Each of these compounds will be crystallized and H_2 sorption isotherms will be recorded. The observation of promising clathrates will lead to the chemical modification of the simple monomers, followed by crystallization and the measurement of H_2 sorption isotherms. The university will also initiate work on compounds with diffuse cavities and prepare and characterize organic crystalline solids with small pores leading to tight, diffuse cavities.

Pacific Northwest National Lab, a partner of this project, will conduct standard simulation methods to fully characterize the structural and thermodynamic properties of H_2 in organic-based clathrates. Modern methods will be used to determine the free energy of formation of both the self-assembled structure and the guest-host system.

Keywords: Hydrogen Storage, Clathrates

99. METAL PERHYDRIDES FOR HYDROGEN STORAGE
$50,000
Michigan Technological University Contact: J. Hwang
DOE Contact: G. Ordaz, (202) 586-8350

The goal of this project is to develop the novel metal perhydride materials with high capacity for hydrogen storage and potential to meet DOE's 2010 hydrogen storage targets. Based on the unique electronic structure of hydrogen atoms and the capability of hydrogen to form hydrogen bonds, bridge bonds and hydrogen clusters, Michigan Technological University conceptualized a novel material, metal perhydrides. Metal perhydrides are different from conventional metal hydrides in that they bind hydrogen clusters rather than individual hydrogen atoms in their molecular structures. Therefore, the hydrogen storage content can be significantly increased. Studies on hydrogen ion clusters indicated that charged species favor the formation of the clusters. Michigan Technological University is looking for the appropriate materials that have charged species to bind hydrogen into clusters. For a proof-of-feasibility study, the University is investigating the reactions between hydrogen and metals. They will also produce testable amount of iron and copper perhydrides and moderate their synthesis and storage conditions; investigate the reaction between the metal hydrides and water; and analyze the hydrogen producing capability. They will also investigate ways to optimize hydrogen storage capacity in these metal perhydride and maximizing the hydrogen release.

Keywords: Hydrogen Storage, Metal Perhydrides

100. HYDROGEN STORAGE MATERIALS WITH BINDING INTERMEDIATE BETWEEN PHYSISORPTION AND CHEMISORPTION
$113,000
A. K. Cheetham/J. Eckert, University of California, Santa Barbara
Partner: Los Alamos National Laboratory, G. Kubas
DOE Technology Development Manager: C. Read, (202) 586-3152

Our approach to the problem of improving the binding strength of hydrogen in hybrid materials includes the use of light metals such as magnesium to support molecular chemisorption of multiple dihydrogen ligands, as well as organic groups with greater charge separation for improved hydrogen binding. In this initial phase of our work on new classes of such materials, we are currently attempting to synthesize new networks for hydrogen adsorption based on oxocarbon dianions. Nearly all of the reported transition metal-oxocarbon structures contain either the squarate or croconate units; there have been no reports of metal deltate (1) compounds, and only two metal rhodizonate (4) compounds exist. Therefore, our work is focused on the attempted synthesis of metal-containing deltate and rhodizonate compounds.

Recently, we also have begun an investigation into the use of di-tert-butyl squarate as a starting material to achieve new metal squarate structures. Previous work in our lab has shown that new open-framework metal phosphate structures can be obtained when organophosphorus compounds are used in place of phosphoric acid. One advantage to using alkylated precursors is that they allow the use of organic solvents or biphasic solvent systems. Our current focus in this area is on the synthesis of squarates of magnesium, which have not been explored previously. These have the potential to be sufficiently lightweight that they can meet the constraints of the DOE storage targets. Work at Los Alamos National Laboratory will focus on preparing materials with Fe centers having multiple dihydrogen ligands, and subsequently anchor these in porous supports. We are particularly interested in extended frameworks of materials containing dicarboxylic acids, such as succinic, glutaric, etc. We have previously made several open-framework materials based upon cobalt(II) and nickel(II) succinates, and there is good reason to believe that the magnesium analogs can be formed. Materials will then be investigated by inelastic neutron scattering studies from the hindered rotational transitions of the sorbed hydrogen molecule in order to determine details of the binding and interaction of hydrogen with our new materials, thereby giving additional direction to our efforts in synthesis. We have previously demonstrated that this technique offers the most detailed and sensitive characterization of guest-host interactions of the adsorbed hydrogen molecule.

Keywords: Hydrogen Storage, Physisorption, Chemisorption, Metal-Organic Compounds

101. NEW CONCEPTS FOR OPTIMIZED HYDROGEN STORAGE IN MOFS
$112,000
O. Yaghi, UCLA/University of Michigan and A. Matzger, University of Michigan
DOE Technology Development Manager: C. Read, (202) 586-3152

The University of Michigan, Ann Arbor proposes to develop new metal-organic framework structures (MOFs) with extremely high surface areas capable of meeting DOE 2010 guidelines. The research also plans to improve mass and volumetric H2 density in MOFs with interpenetration and inclusion strategies. Michigan will implement three major strategies that minimize open space while increasing total surface area for H2 binding. Initially, they will use linkers with exposed edges, resulting in ultra-high surface area MOFs. A prototypical example is MOF-177. They will also take these frameworks and impregnate the large pores with guests designed to adsorb hydrogen. Finally, catenation will be explored as a strategy to decrease open space not participating in gas binding. To explore these approaches, equilibrium H2 uptake will be determined as a function of structure under DOE 2010 targets. Raman spectroscopy, inelastic neutron scattering, and modeling will be employed to aid in these efforts.

Keywords: Hydrogen Storage, Metal-Organic Framework

102. A RADICALLY NEW METHOD FOR HYDROGEN STORAGE IN HOLLOW GLASS MICROSPHERES
$100,000
Alfred University Contact: J. Shelby
Partners: MoSci Corp, Savannah River National Laboratory
DOE Contact: G. Ordaz, (202) 586-8350

The primary goal of this project is to demonstrate that a working hydrogen storage and release device can be produced using the newly discovered phenomenon of photo-enhanced hydrogen diffusion in glasses. Therefore, the project will seek to demonstrate that the:

- Hollow glass microspheres (HGMS) of the desired composition and quality can be produced
- HGMS can be filled to sufficient pressure to meet the DOE hydrogen storage targets
- The photo-induced diffusion effect can be used to release hydrogen at a sufficient rate for transportation applications
- This technology can be demonstrated at the "bench-top" level

Alfred University will conduct a basic scientific study that will provide an understanding of the mechanism(s) which lead to photo-enhanced hydrogen diffusion in glasses. This information will be used to optimize the application of photo-enhanced hydrogen diffusion in glasses to a working device.

Alfred University and its partner MoSci Corp will develop the technology necessary to produce HGMS of the desired composition and quality in sufficient quantities to provide proof-of-concept of the storage method. Alfred University and its other partner Savannah River National Laboratory will also fill the HGMS with high pressure hydrogen and determine the parameters necessary for the high pressure filling and monitor their behavior during repeated filling to high pressures.

Keywords: Hydrogen Storage, Glass Microspheres

INDUSTRIAL TECHNOLOGIES PROGRAM

	FY 2005
INDUSTRIAL TECHNOLOGIES PROGRAM TOTAL	$46,683,836
ALUMINUM SUBPROGRAM	$1,940,478
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$100,000
Microwave Assisted Electrolytic Cell	100,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,270,445
Surface Behavior of Aluminum Alloys Deformed under Various Processing Conditions	32,549
Low Temperature Reduction of Alumina Using Fluorine Containing Ionic Liquids	96,258
Effect of Impurities on the Processing of Aluminum Alloys in Casting, Extrusion, and Rolling	50,000
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	750,000
Improved Energy Efficiency in Aluminum Melting	135,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$570,033
Spray Rolling Aluminum Strip	250,000
Degassing of Aluminum Alloys Using Ultrasonic Vibrations	60,000
Effect of Casting Conditions & Composition on Microstructural Gradients in Roll Cast Aluminum Alloys	93,034
Energy Efficient Isothermal Melting of Aluminum	76,999
Continuous Severe Deformation Processing of Aluminum Alloys	90,000
METAL CASTING SUBPROGRAM	$819,468
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$240,000
Development of Elevated Temperature Aluminum MMC Alloy	90,000
Development of Surface Engineered Coatings for Die Casting Dies	150,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING	$579,468
Corrosion Testing Practices for High Alloys	90,000
Advanced Lost Foam Casting Technology	240,000
Development of CCT Diagrams for High Alloys Steels	75,000
Improved Die Casting Process to Preserve the Life of the Inserts	90,000
Characterization of Surface Anomalies from Magnetic Particle and Liquid Penetrant Indications	84,468

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2005
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	$11,008,944
Research Related to the Development of the Automated Steel Cleanliness Analysis Tool (ASCAT)	1,992,318
Enhanced Inclusion Removal from Steel in the Tundish	860,880
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	407,699
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	1,165,125
Characterization of Fatigue and Stress/strain Behavior in Advanced High Strength Steels	385,221
Validation of Hot Strip Mill Model	2,935,214
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	$8,433,398
Ironmaking Challenge - The Mesabi Nugget Research Project	5,555,008
Development of Steel Foam Materials and Structures	754,279
Generation of Next Generation Heating System for Scale Free Steel Reheating	1,106,337
New Generation Metallic Iron Nodule Technology in Electric Furnace Steelmaking	1,017,774
MATERIALS SUBPROGRAM	$8,505,000
DEGRADATION RESISTANT MATERIALS	$6,105,000
MATERIALS DEVELOPMENT AND PROCESSING	$541,000
Development of Stronger and More Reliable Cast Austenitic Stainless Steels (H-series)\ Based on Scientific Design Methodology	100,000
Low-temperature Surface Carburizing of Stainless Steels	366,000
Development of a New Class of Fe-3Cr-W(V) Ferritic Steels for Industrial Process Applications	75,000

[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 FY05 funding data are not available.

INDUSTRIAL TECHNOLOGIES PROGRAM (continued)

	FY 2005
MATERIALS SUBPROGRAM (continued)	
DEGRADATION RESISTANT MATERIALS (continued)	
ULTRA-HARD MATERIALS	$1,654,651
Novel Superhard Materials and Nanostructured Diamond Composites for Multiple Industrial Applications	338,000
Development of Bulk Nanocrystalline Cemented WC for Industrial Applications	445,141
Crosscutting Industrial Applications of a New Class of Ultra-Hard Borides	216,510
Development of Ultrananocrystalline Diamond (UNCD) Coatings for SiC Multipurpose Mechanical Pump Seals	655,000
WEAR/CORROSION RESISTANT MATERIALS	$2,487,000
Advanced Composite Coatings for Industries of the Future	315,000
Advanced Wear and Corrosion Resistant Systems Through Laser Surface Alloying	135,000
Alkaline-resistant Fe-phosphate Glass Fibers as Concrete Reinforcement	267,000
Development of Functionally Graded Materials for Manufacturing Tools	705,000
Development of Materials Resistant to Metal Dusting	410,000
Stress-assisted Corrosion in Boiler Tubes	70,000
Structurally Integrated Coatings for Wear and Corrosion	585,000
THERMOPHYSICAL DATABASES AND MODELING	$1,272,349
Thermochemical Models and Databases for High Temperature Materials Processing and Corrosion	535,000
Development of Combinatorial Methods for Alloy Design and Optimization	40,000
Prediction of Corrosion of Advanced Materials and Fabricated Components	697,349
MATERIALS FOR SEPARATIONS	$150,000
Novel Modified Zeolites for Energy-Efficient Hydrocarbon Separations	150,000
MATERIALS FOR ENERGY SYSTEMS	$2,400,000
REFRACTORIES/HEAT RECOVERY	$1,925,000
Advanced Thermoelectric Materials for Effective Waste Heat Recovery in Process Industries	520,000
Materials for High-temperature Black Liquor Gasification	550,000
Multifunctional Metallic and Refractory Materials for Handling of Molten Metals	390,000
Materials for Industrial Heat Recovery Systems	465,000
WELDING/JOINING	$475,000
Advanced Integration of Multi-scale Mechanics and Welding Process Simulation in Weld Assessment	475,000

INDUSTRIAL TECHNOLOGIES PROGRAM

ALUMINUM SUBPROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

103. MICROWAVE ASSISTED ELECTROLYTIC CELL
$100,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

104. SURFACE BEHAVIOR OF ALUMINUM ALLOYS DEFORMED UNDER VARIOUS PROCESSING CONDITIONS
$32,549
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

105. LOW-TEMPERATURE REDUCTION OF ALUMINA USING FLUORINE CONTAINING IONIC LIQUIDS
$96,258
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

106. EFFECT OF IMPURITIES ON THE PROCESSING OF ALUMINUM ALLOYS
$50,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

107. COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACH FOR THE DESIGN OF MOLD SURFACE TOPOGRAPHY
$100,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

108. MOLTEN ALUMINUM TREATMENT BY SALT FLUXING WITH LOW ENVIRONMENTAL EMISSIONS
$106,638
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

109. INERT METAL ANODES FOR PRIMARY ALUMINUM PRODUCTION
$750,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

110. IMPROVED ENERGY EFFICIENCY IN ALUMINUM MELTING
$135,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

111. SPRAY ROLLING ALUMINUM STRIP
$250,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493
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, Sheet

112. DEGASSING OF ALUMINUM ALLOYS USING ULTRASONIC VIBRATIONS
$60,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

Keywords: Ultrasonic, Degassing, Casting

113. EFFECT OF CASTING CONDITIONS AND COMPOSITION ON MICROSTRUCTURAL GRADIENTS IN ROLL CAST ALUMINUM ALLOYS
$93,034
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

Keywords: Microstructural, Alloys, Casting, Annealing

114. ENERGY EFFICIENT ISOTHERMAL MELTING OF ALUMINUM
$76,999
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

Keywords: Isothermal Melting Process, Immersion Heater, Refractory

115. CONTINUOUS SEVERE PLASTIC DEFORMATION PROCESSING ALUMINUM ALLOYS
$90,000
DOE Contact: Ehr Ping Huangfu, (202) 586-1493

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

METAL CASTING SUBPROGRAM

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

116. DEVELOPMENT OF ELEVATED TEMPERATURE ALUMINUM MMC ALLOY
$90,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Eck Industries, Inc. Contact: Dave Weiss, (920) 682-4618 x108

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

117. DEVELOPMENT OF SURFACE ENGINEERED COATINGS FOR DIE CASTING DIES
$150,000
DOE Contact: Ehr Ping HuangFu, (202) 586-1493
Colorado School of Mines Contact: John Moore, (303) 273-3770

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

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, OR TESTING

118. CORROSION TESTING PRACTICES FOR HIGH ALLOYS
$90,000
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

119. ADVANCED LOST FOAM CASTING TECHNOLOGY
$240,000
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

120. DEVELOPMENT OF CCT DIAGRAMS FOR HIGH ALLOY STEELS
$75,000
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

121. IMPROVED DIE CASTING PROCESS TO PRESERVE THE LIFE OF THE INSERTS
$90,000
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

122. CHARACTERIZATION OF SURFACE ANOMALIES FROM MAGNETIC PARTICLES AND LIQUID PENETRANT INDICATIONS
$84,468
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; and evaluate the effectiveness of current surface quality standards in predicting the actual size and shape of the indication and their effect on casting performance.

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

STEEL SUBPROGRAM[1]

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

123. 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. Completed in FY05.

Keywords: Thermomechanical Processing, Modeling, Microstructure

124. 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: Ever Barbero

The objectives of this project are to develop new bulk materials and surface treatment/coatings for life improvement of molten metal bath hardware and bearings in continuous hot-dip processes used for coating steel strip. The project goal is to result in extension of component life by an order of magnitude. Major progress has been made in developing materials to increase the life of molten zinc pot hardware on steel galvanizing lines by a factor of ten. Interest in this project is high because these high-speed hot dip lines often experience catastrophic component failures requiring shut down of the line. Steel industry hot dip operators are collaborating with researchers from West Virginia University, the Lead Zinc Research Organization Inc., and Oak Ridge National Laboratory. Completed in FY05.

Keywords: Pot Hardware, Hot Dip Processing, Lifetime

125. 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. Completed in FY03.

Keywords: Electrolytic Tin Plate, Passivation, Chromium-Free

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

126. 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

[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 FY05 funding data are not available.

5) introduction of ASCAT as part of the steel production process in the steel mill environment. Completed in FY05.

Keywords: Steel, Automation, Cleanliness Analysis

127. ENHANCED INCLUSION REMOVAL FROM STEEL IN THE TUNDISH
$860,880
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

128. 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
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. Completed in FY04.

Keywords: High-Strength Steels, Variability

129. 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. Completed in FY05.

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

130. CLEAN STEEL - ADVANCING THE STATE OF THE ART
$407,699
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. Completed in FY04.

Keywords: Steel, Inclusion Removal

131. 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. Completed in FY03.

Keywords: High-Strength Steels, Formability

132. DEVELOPMENT OF A STANDARD METHODOLOGY FOR QUANTITATIVE MEASUREMENT OF STEEL PHASE TRANSFORMATION KINETICS AND DILATION STRAINS USING DILATOMETRIC METHODS
$1,165,125
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). Completed in FY04.

Keywords: Steel, Transformation, Dilatometer, Gleeble

133. 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. Completed in FY03.

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

134. VALIDATION OF HOT STRIP MILL MODEL
$2,935,214
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. Completed in FY05.

Keywords: Steel, Hot Strip Mill, Modeling

135. 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

136. 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. Completed in FY05.

Keywords: High-Strength Steels, Spot Welding

MATERIALS PREPARATION, SYNTHESIS DEPOSITION, GROWTH OR FORMING

137. 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. Completed in FY05.

Keywords: Ironmaking, Rotary Hearth, Mesabi Nugget Project

138. DEVELOPMENT OF STEEL FOAM MATERIALS AND STRUCTURES
$754,279
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 percent to below 1.0 percent while maintaining densities at 50 percent and lower. This has also enabled the development of more useful microstructures that will yield better properties. Improvements in forming and processing have produced a more spherical pore shape and uniform pore size distribution in the foamed steel that will perform in a more predictable and consistent manner. Simple geometry components have been produced. A mechanical and physical properties database is being built that will allow design and application of lightweight steel with a controlled pore structure. Completed in FY05.

Keywords: Steel, Foam, Powder Metallurgy

139. GENERATION OF NEXT GENERATION HEATING SYSTEM FOR SCALE FREE STEEL REHEATING
$1,106,337
DOE Contact: Simon Friedrich, (202) 586-6759
E3M Contact: Arvind Thekdi, (240) 715-4333

The overall objective is to develop and test a scale free heating system that reduces scale formation in steel reheating process resulting in substantial reduction in energy use, improvement in steel quality and significant cost advantages for the U.S. steel industry. The project will be carried out in two phases. The primary objective for Phase I is to develop concept and heating system for a process to achieve scale free heating using non-oxidizing furnace atmosphere generated through sub-stoichiometric (fuel rich) combustion of fuel within the furnace itself. A go/no-go decision will be made through the use of critical performance parameters and criteria to proceed to Phase II. Objectives of Phase II are research and development for experimental proof of concept for scale free heating, chemical heat recovery system design and detail cost-benefit analysis and its evaluation by the steel industry partners to make a go/no-go decision for field testing of the system and further commercialization strategy.

Keywords: Steel, Reheating

140. NEW GENERATION METALLIC IRON NODULE TECHNOLOGY IN ELECTRIC FURNACE STEELMAKING
$1,017,774
DOE Contact: Simon Friedrich, (202) 586-6759
University of Minnesota Contact: Donald A Fosnacht, (218) 720-4282

This project expands upon previous research conducted at the University of Minnesota Duluth's Natural Resources Research Institute and offers alternative process methodologies to those reported by Kobe and JFE Steel. Three major issues have been identified and will be addressed in this project for producing high quality metallized iron nodules (MIN) at low cost: 1) reduce the process operating temperature, 2) control the furnace gas atmosphere over the MIN, and 3) effectively use sub-bituminous coal as the reductant. The project will be conducted in two Phases. In Phase I, preliminary studies will be completed to define furnace atmosphere control modifications and how to incorporate sub-bituminous coal in the process. In Phase II, the pilot linear hearth furnace will be midified and used to conduct tests to implement modifications identified in Phase I, and to establish base processing conditions that should be utilized in engineering a commercial size iron nodule production system. After Phase I, there is a go/no-go decision point before proceeding to Phase II.

Keywords: Steel, Electric Furnace, Iron Nodule

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 2005 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

141. DEVELOPMENT OF STRONGER AND MORE RELIABLE CAST AUSTENITIC STAINLESS STEELS (H-SERIES) BASED ON SCIENTIFIC DESIGN METHODOLOGY
$100,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: Sharon Robinson, (865) 574-6779

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

142. LOW-TEMPERATURE SURFACE CARBURIZING OF STAINLESS STEELS
$366,000
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

143. DEVELOPMENT OF A NEW CLASS OF Fe-3Cr-W(V) FERRITIC STEELS FOR INDUSTRIAL PROCESS APPLICATIONS
$75,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: Sharon Robinson, (865) 574-6779

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

ULTRA-HARD MATERIALS

144. NOVEL SUPERHARD MATERIALS AND NANOSTRUCTURED DIAMOND COMPOSITES FOR MULTIPLE INDUSTRIAL APPLICATIONS
$338,000
DOE Contact: Sara Dillich, (202) 586-7925

Researchers at Los Alamos National Laboratory, the Carnegie Institution’s Geophysical Laboratory, and the Phoenix Crystal Corporation have produced synthetic single crystal diamonds which are harder than natural diamond. The gem-sized crystals were produced at a rate up to 100 times faster than other methods used to date. Diamond single crystals were grown using high-growth rate microwave plasma chemical vapor deposition (CVD), in which hydrogen gas and methane are bombarded with charged particles or plasma in a chamber. The crystals were then processed at high-pressure, high-temperature conditions to harden them further. The crystals are anticipated to have a variety of industrial applications including high-pressure anvils, electronic devices and cutting tools. Results have been reported in the February 20th online Physica Status Solidi. IMF estimates that this project will save approximately 0.7 TBtu/year by 2020.

Keywords: Single Crystal Diamond, Chemical Vapor Deposition, Hard Materials

145. DEVELOPMENT OF BULK NANOCRYSTALLINE CEMENTED WC FOR INDUSTRIAL APPLICATIONS
$445,141
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
$216,510
OE 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
$655,000
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
$315,000
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
$135,000
DOE Contact: Sara Dillich, (202) 586-7925
Applied Research Laboratory, Pennsylvania State University Contact: R. P. Martukanitz

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
$267,000
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
$705,000
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
$410,000
DOE Contact: Sara Dillich, (202) 586-7925
Materials Technology Institute Contact: Emory Ford

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. STRESS-ASSISTED CORROSION IN BOILER TUBES
$70,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: Sharon Robinson, (865) 574-6779

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

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

154. STRUCTURALLY INTEGRATED COATINGS FOR WEAR AND CORROSION
$585,000
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

155. THERMOCHEMICAL MODELS AND DATABASES FOR HIGH TEMPERATURE MATERIALS PROCESSING AND CORROSION
$535,000
DOE Contact: Sara Dillich, (202) 586-7925

Sandia National Laboratory and Oak Ridge National Laboratory are working with nine industrial partners on a project to improve the availability, accuracy and accessibility of thermochemical property data that is required to understand, simulate and optimize industrial processes. Project accomplishments and milestones center on developing thermodynamic models of condensed-phase systems, prediction of high-temperature thermochemistry of gas-phase species, and the development of a Web-based database/model site that will provide the necessary input for commercial operation. The database is now available at: http://www.ca.sandia.gov/HiTempThermo/index.html. Presently, the database contains information for gas-phase compounds and a wide range of metal oxides used in refractories. Data on this site enable the modeling of materials and refractories in high-temperature industrial environments, so that both optimal selection of compatible materials, as well as interpretation of failure mechanisms can occur. Project activities are directed toward predicting thermodynamic data for compounds of relevance to the glass, pulp/paper, chemicals and metals refining industries, all of which use refractories extensively. Currently, the database has more than 70 industrial and academic subscribers and the site has received over 3,300 hits since its inception more than a year ago. IMF estimates that this project will save approximately 1.4 TBtu/year by 2020.

Keywords: Thermochemical Data, Gas-Phase Compounds, Metal Oxides, Industrial Processes

156. DEVELOPMENT OF COMBINATORIAL METHODS FOR ALLOY DESIGN AND OPTIMIZATION
$40,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: Sharon Robinson, (865) 574-6779

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

157. PREDICTION OF CORROSION OF ADVANCED MATERIALS AND FABRICATED COMPONENTS
$697,349
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

158. NOVEL MODIFIED ZEOLITES FOR ENERGY-EFFICIENT HYDROCARBON SEPARATIONS
$150,000
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

159. ADVANCED THERMOELECTRIC MATERIALS FOR EFFECTIVE WASTE HEAT RECOVERY IN PROCESS INDUSTRIES
$520,000
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

160. MATERIALS FOR HIGH-TEMPERATURE BLACK LIQUOR GASIFICATION
$550,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: James Keiser, (865) 574-4453

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 percent. 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

161. MULTIFUNCTIONAL METALLIC AND REFRACTORY MATERIALS FOR HANDLING OF MOLTEN METALS
$390,000
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

162. MATERIALS FOR INDUSTRIAL HEAT RECOVERY SYSTEMS
$465,000
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

163. ADVANCED INTEGRATION OF MULTI-SCALE MECHANICS AND WELDING PROCESS SIMULATION IN WELD ASSESSMENT
$475,000
DOE Contact: Sara Dillich, (202) 586-7925
ORNL Contact: Sharon Robinson, (865) 574-6779

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

SOLAR ENERGY TECHNOLOGY PROGRAM

	FY 2005
SOLAR ENERGY TECHNOLOGY PROGRAM TOTAL	$85,768,000[1]
OFFICE OF SOLAR ENERGY TECHNOLOGIES	$67,214,000
NATIONAL PHOTOVOLTAICS PROGRAM	$67,214,000[2]
PHOTOVOLTAICS RESEARCH & DEVELOPMENT	$61,524,000[3]
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, AND FORMING	$16,781,000
Thin-Film Amorphous Silicon and Thin-Film Polycrystalline Materials for Solar Cells	12,906,000
Deposition of III-V Semiconductors for High-Efficiency Solar Cells	2,975,000
Nanocrystalline and Organic Solar Cell Materials	900,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, AND TESTING	$7,630,000
Materials and Device Characterization	6,230,000
Materials Structure and Composition	1,400,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR, AND TESTING	$4,227,000
Materials Improvement for High-Efficiency Crystalline Silicon Solar Cells	2,260,000
Instrumentation and Facilities	1,967,000

[1]This is the total funding for SETP, including materials and other activities.

[2]This is the total funding for the National Photovoltaics Program, including materials and other activities.

[3]This is the total funding for photovoltaics research and development, including materials and other activities.

SOLAR ENERGY TECHNOLOGY PROGRAM

OFFICE OF SOLAR ENERGY TECHNOLOGIES

The Photovoltaics Subprogram of the Solar Energy Technologies Program (SETP) sponsors research and development with the goal of making terrestrial solar photovoltaic (PV) 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 (2005 dollars) of approximately $0.05-$0.10/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 wafer separation, the complexity of junction formation and cell fabrication, and the material and labor 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 (and domestic) photovoltaic module production is dominated by crystalline silicon technology. However, the percentage of modules in the United States made from thin-film technologies is steadily increasingly.

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), minority carrier lifetime, and device engineering factors. Spectral response is limited by non-absorption of sub-bandgap photons. Collection of energetic photons is limited by thermalization of “hot” carriers through lattice scattering. Minority carrier lifetime is limited by the introduction of quantum states resulting from material defects. Engineering factors include cell thickness, junction depth, reflection coefficient, parasitic resistances (i.e., high series resistance in the metallization and contacts, low shunt resistance through the thickness of the cell), and passivation of 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. There are also several subcontracts for the development of potentially very inexpensive polymer solar cells. The SETP effort is also concerned with advanced materials that enhance module reliability.

NATIONAL PHOTOVOLTAICS PROGRAM

MATERIAL PREPARATION, SYNTHESIS, DEPOSITION, GROWTH, AND FORMING

164. THIN-FILM AMORPHOUS SILICON, AND THIN-FILM POLYCRYSTALLINE MATERIALS, FOR SOLAR CELLS
$12,906,000
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 is development of technologies for 15 percent efficient (stabilized) photovoltaic modules with cost under $50/m^2 and with 30-year lifetime. The long-term goal for polycrystalline thin films includes 25% efficient multijunction cells, and subsequent 20% efficient large-area modules. These achievements will allow system lifetime user energy cost of approximately $0.05 - $0.10 / kWh, and subsequent wide competition of thin-film photovoltaics for large-scale distributed power generation.

Thin-Film Amorphous Silicon: These projects perform research on the deposition and characterization of amorphous and nanocrystalline silicon thin films to improve solar cell conversion efficiency while maintaining 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 can be deposited by plasma enhanced chemical vapor deposition (glow discharge), thermal chemical vapor deposition (hot wire), 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, by investigating alternate window layer materials, 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.

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

165. DEPOSITION OF III-V SEMICONDUCTORS FOR HIGH-EFFICIENCY SOLAR CELLS
$2,975,000
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 over 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 can be deposited by metal organic chemical vapor deposition (MOCVD), liquid phase epitaxy, and molecular beam epitaxy (MBE). NREL has verified a monolithic two-terminal three-junction III-V cell at over 37 percent conversion efficiency under high concentration.

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

166. NANOSTRUCTURE AND ORGANIC SOLAR CELL MATERIALS
$900,000
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 for electrochemical solar cells), 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 solar cells. Fundamental research explores the physical and chemical mechanisms of these novel photovoltaic materials, and identifies the limits to efficiency and future commercial viability. One subcontract explores the possible development of nanocrystalline films for electrochemical solar cells employing impact ionization to achieve internal quantum efficiencies >1.

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION, AND TESTING

167. MATERIALS AND DEVICE CHARACTERIZATION
$6,230,000
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. These measurements allow study of critical material parameters such as doping impurities, crystallographic mismatch, and other defects that limit photovoltaic performance. 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, Electron Microscopy, SIMS, Auger Spectroscopy, Minority Carrier Lifetime, Semiconductor Defects, Solar Cell Testing, Module Testing, Photovoltaic Material Characterization

168. MATERIALS STRUCTURE AND COMPOSITION
$1,400,000
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 longer 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 complicated alloys, e.g., GaInAsN, impurity precipitation and dissolution in crystalline silicon, structure of defect sites in silicon materials, and mechanism 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, AND TESTING

169. MATERIALS IMPROVEMENT FOR HIGH-EFFICIENCY CRYSTALLINE SILICON SOLAR CELLS
$2,260,000
DOE Contact: Jeffrey Mazer, (202) 586-2455
NREL Contacts: David Mooney, (303) 384-6782,
Bhushan Sopori, (303) 384-6683, 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 commercially-compatible processes. 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 Crystalline Silicon Workshop on Solar Cell Materials and Processes, which is 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. A major goal 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 Czochralski growth.

Keywords: Crystalline Silicon, Multicrystalline Silicon, Silicon Ribbon, 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, Crystalline Silicon Workshop

170. INSTRUMENTATION AND FACILITIES
$1,967,000
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NREL Contact: Pete Sheldon, (303) 384-6533,
Larry Kazmerski, (303) 384-6600
SNL Contact: Jeff Nelson, (505) 284-1715

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

Major work is progressing on the new Science & Technology Facility (S&TF) which is being built next to the SERF Building at NREL (Golden, CO). The S&TF construction will be finished by mid-CY 2006, and most move-in procedures will be completed by the end of CY 2006. The first major system in the S&TF will be a world-class multi-chambered cluster tool for the characterization of silicon processes and silicon photovoltaic devices.

Keywords: Solar Cell Characterization, Photovoltaic Characterization, Semiconductor Measurement, Semiconductor Characterization, Semiconductor Materials Measurement, Semiconductor Equipment, Fourier Transform Spectroscopy, Electron Microscopy, MBE, MOCVD, Silicon Cluster Tool, Solar Cells

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

	FY 2005
HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS TOTAL	$36,000,000
Second Generation Wire Development	6,850,000
Systems Technology - Partnerships with Industry	19,850,000
Strategic Research	9,300,000

OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

HIGH TEMPERATURE SUPERCONDUCTIVITY FOR ELECTRIC SYSTEMS

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

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

Systems research and development activities focus on the research, development, and testing of prototype HTS power system applications through industry-led projects. Research teams investigate adaptability issues for using superconducting wire in power system applications, which include transmission cables, generators, transformers, fault-current limiters, and flywheel electricity systems. In addition, program efforts target end-user applications in energy-intensive industries, including large electric motors (over 5000 HP), 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 2005, the Superconductivity Program's parent organization transitioned from the Office of Electric Transmission and Distribution to the Office of Electricity Delivery and Energy Reliability (OE). OE'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:

<u>Energy Policy Act of 2005</u>: The development and use of high-temperature superconductors to enhance the reliability, operational flexibility, or power carrying capability of the electric transmission or distribution systems; or increase the efficiency of electric energy generation, transmission, distribution, or storage systems.

<u>National Energy Policy (2001)</u>: Expand the Department's research and development on transmission reliability and superconductivity

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

<u>President's Council of Advisors on Science and Technology (2002)</u>: 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.

<u>Grid 2030 (2003)</u>: 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 2005 annual operating budget of High Temperature Superconductivity for Electric Systems Program was slightly higher than the prior year's budget. Results that will be presented at the Peer Review in the summer of 2006 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

171. SECOND GENERATION WIRE DEVELOPMENT
$6,850,000
National Laboratories:
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

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. Researchers are undertaking the characterization of microstructural and superconducting properties of second generation wire to improve understanding of Jc-limiting factors relating to formation and growth kinetics of high-temperature 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. Research continues to develop strengthened and conductive Cu-based substrates with good texture.

IBAD Research - Teams continue research to scale up IBAD MgO process to long lengths with uniform texture. IBAD MgO offers significant cost benefits compared to IBAD YSZ. In 2005, 135 m IBAD MgO tapes were fabricated on 50 micron thick substrates at 10 m/h. By using a helix tape handling system, a tape speed of 10 m/h was achieved to produce IBAD MgO with texture of 6.4˚.

YBCO/RABiTS - Efforts continue to develop an all-solution buffer/YBCO process to fabricate lower cost high performance second generation coated conductors with an I_C of 300 A/cm. Alternative architectures with simplified layers comprised of multi-functional buffers deposited by industrially scalable methods are being investigated.

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

172. SYSTEMS TECHNOLOGY - PARTNERSHIPS WITH INDUSTRY
$19,850,000

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:

SPI READINESS REVIEW PROGRAM

The focus of this project is on collaboration with the SPI teams 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.

ORNL Contact: Mike Gouge, (865) 576-4467

TRIAXIAL COLD DIELECTRIC SUPERCONDUCTING DISTRIBUTION CABLE – COLUMBUS OHIO PROJECT

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. Off-line testing in Columbus, Ohio will take place from May-July 2006 to test long length HTS cable under real environmental stresses and electric loads. The system will form an important electrical link in a utility substation in Columbus Ohio replacing conventional cables with a limited current-carrying capacity. The project is partnered with Ultera, utility partner: AEP, Bixby substation, using 13.2 kV, load rating 3.0 kV, 69 MVA, triax cable design, cold dielectric, splice, underground, multiple 90 degree bends, length 330 m.

Ultera Contact: David Lindsay, (770) 832-4916

COLD DIELECTRIC SUPERCONDUCTING DISTRIBUTION CABLE (WITH YBCO SEGMENT) – ALBANY CABLE PROJECT

This project is partnered with utility Niagara Mohawk, SuperPower, BOC, Sumitomo Electric, and New York State Energy Research and Development Authority. The purpose involves the development and demonstration of a High Temperature Superconducting cable installation between two major substations and splice. This one of a kind demonstration includes the usage of second generation wire cable voltage 34.5 kV, load rating 800 A, 48 MVA, cold dielectric, cable design incorporating YBCO, length 350 m.

SuperPower Contact: Chuck Weber, (518) 346-1414

COAXIAL COLD DIELECTRIC SUPERCONDUCT-ING TRANSMISSION CABLE – LIPA PROJECT

The primary objective of this project involves the demonstration of a High Temperature Superconductor (HTS) power cable in the Long Island Power grid, this project spans nearly half a mile and will serve as a permanent link in the Long Island Power Authority's (LIPA) grid network. The installation will represent the first-ever superconductor cable in a live grid at transmission voltages of 138 kV, 2400 A, 600 MVA, design fault current 69 kA at 250 ms (15 line cycles), coaxial cold dielectric design, 3-phase, to be installed between two major substations, length 610 m.

LIPA Contact: Tom Welsh, (516) 545-3162

HTS TRANSFORMER

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.

ORNL Contact: Shirish Mehta, (262) 547-0121

DEVELOPMENT OF ULTRA-EFFICIENT HTS MOTOR SYSTEM

The purpose of the project is to perform research and development related to commercial viability of industrial motors with high temperature superconducting (HTS) windings. The R&D areas identified were 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.

Rockwell Automation Contact: Rich Schiferl, (216) 261-3644

DESIGN AND DEVELOPMENT OF A 100 MVA HTS GENERATOR

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.

GE Contact: James Fogarty, (518) 385-4142

DEVELOPMENT STATUS OF FLYWHEEL ELECTRICITY SYSTEM

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.

Boeing Contact: Mike Strasik, (425) 237-7176

MATRIX FAULT CURRENT LIMITER

The purpose of this project is to conduct R&D on specified components and provide technical design support to a SuperPower, Inc. This device incorporates a series-parallel array of bulk HTS elements and inductors in a sub-cooled liquid nitrogen 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. The main focus of current R&D fall into three general areas: general design, cryogenic cooling, and high voltage subsystem design.

SuperPower Contact: Philip Pellegrino, (518) 346-1414

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

173. STRATEGIC RESEARCH
$9,300,000
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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
Idaho Operations Office (University Strategic Research) Contact: John Yankeelov,
(208) 526-7049
Oxford Superconducting Technology Contact:
Seung Hong, (732) 541-1300
University of Wisconsin Contact:
David C. Larbalestier, (608) 263-2194

Strategic Research is dedicated to investigating new approaches in producing or analyzing superconductivity and HTS applications. This research focuses on high-risk concepts that show promise in the long-term, but additional research is needed before such concepts could interest the private sector. The focus is on solving potential fabrication problems to be encountered in new coated conductors and in HTS application subsystems. 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 2005. A variety of deposition and processing strategies were being investigated to develop a fundamental understanding of this deposition approach and to optimize film properties.

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. In 2005, one research focus has been design and engineering for low ac loss, flux pinning, and reasons behind the dependence of the transverse stress on RABiTS substrate materials. Other R&D efforts have been directed towards understanding the development of high Ic ex-situ processes rare earth substitutions of coated conductors

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.

Thick HTS films - Teams intend to increase the deposition rates of both IBAD and HTS films with extending film thickness and reducing ac losses to enable higher current carrying ability. They will address the process of in-situ scale-up transfers to metal tapes. Collaborations with partners will proceed in 2005 in order to investigate methods that will increase performance and reduce costs of IBAD technology.

Process technology - DOE partners worked toward developing and demonstrating process technology needed for epitaxial growth of buffer layers. 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. Other efforts will address the process of in-situ scale-up transfers to metal tapes.

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 2005
OFFICE OF SCIENCE GRAND TOTAL	$741,868,297
OFFICE OF BASIC ENERGY SCIENCES	$686,700,000
DIVISION OF MATERIALS SCIENCES AND ENGINEERING	$247,914,000
Theoretical Condensed Matter Physics	19,798,000
Experimental Condensed Matter Physics	42,631,000
Materials Chemistry	46,860,000
Mechanical Behavior and Radiation Effects	14,008,000
X-ray and Neutron Scattering	46,061,000
Structure and Composition of Materials	24,907,000
Physical Behavior	25,551,000
Synthesis and Processing Sciences	15,149,000
Engineering Physics	5,306,000
Experimental Program to Stimulate Competitive Research	7,643,000
DIVISION OF SCIENTIFIC USER FACILITIES	$438,786,000
X-ray and Neutron Scattering Facilities	326,326,000
Nanoscience Centers	112,460,000
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH	$45,369.297
TECHNOLOGY RESEARCH DIVISION	$45,369,297
SMALL BUSINESS INNOVATION RESEARCH PROGRAM	$42,948,439
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$9,462,210
FY 2005 PHASE I	$1,691,166
Very High Temperature (400+ C), High Power Density Silicon Carbide (SiC) Power Electronic Converters	99,989
Universal Converter Using Silicon Carbide	99,814
A New Scintillator for Time-of-Flight PET	100,000
High Efficiency, Low Cost Scintillators for PET	100,000
A Very High Spatial Resolution Detector for Small Animal PET	100,000
High-Temperature Ceramic Capacitors for Applications in Deep Drilling and Completion Processes	99,998
Abuse Tolerant, Voltage Stabilized Li-ion Cell	100,000
Organic Additives as Redox Shuttles for Overcharge Protection of Lithium Ion Batteries	99,979
Improved Low-Temperature Performance of Safer, Low-Cost Lithium Iron Phosphate Cathodes for Lithium-Ion Batteries	99,315
Safer, Non-Toxic, Alternative Electrolytes	92,175
Novel Large Area High Resolution Neutron Detector for the Spallation Neutron Source	100,000
Extreme Environment Control Sensors	99,963
Refractory Substrate/Capillary Assisted/Thin Flowing Lithium Film Plasma Facing Component	99,953
Innovative Nanoparticle Insulation Systems for Fusion Magnets	99,985
Modified Epoxy Resin Systems as Composite Insulation in Fusion Confinement Systems	99,998
Fabrication of Complex Copper Cooling Devices Using Ultrasonic Metal Consolidation to Locally Cool and Monitor High Energy Electron Sources	99,998
Cost-Effective, High-Performance, High-Purity Niobium Superconducting Radio Frequency Cavities	99,999

OFFICE OF SCIENCE (continued)

	FY 2005
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
TECHNOLOGY RESEARCH DIVISION (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING (continued)	
FY 2005 PHASE II (FIRST YEAR)	$3,699,764
Novel Silica Aerogel Panels as Radiators for Cherenkov Detectors	350,000
Single Crystal Molybdates for Neutrinoless Double Beta Decay Experiments	350,000
Nanocomposite Polymers for Smart Window Films	375,000
Enhancing Charge Injection and Device Integrity in Organic LEDs	374,971
Zinc Oxide Based Light Emitting Diodes	375,000
High Efficiency, White TOLEDs for Lighting Applications	375,000
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	374,874
Novel Heat Exchangers with Enhanced Surface	374,992
Composite, High-Temperature Seals for Gas Separation Membrane Devices	374,928
Optimization of Metal Alloy for High Pressure Hydrogen Separation Membrane	374,999
FY 2005 PHASE II (SECOND YEAR)	$4,071,280
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
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,393,818
FY 2005 PHASE I	$499,687
High Throughput Microcantilever-Based Detection of Antigen-Antibody Binding	99,954
Evaluation of Nuclear Grade SiC/SiC Composites for Control Rod Sheaths	99,971
Nanotechnology Enabled Advanced Industrial Heat Transfer Fluids	99,995
Micro/Nano-Encapsulation of Partial Oxidation Biocatalysts	99,999
Improvement of the Properties of Tubular Internal-Tin Nb_3Sn	99,768

OFFICE OF SCIENCE (continued)

	FY 2005
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
TECHNOLOGY RESEARCH DIVISION (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
FY 2005 PHASE II (FIRST YEAR)	$1,776,934
Innovative, Low Cost, Radiation-Resistant Fusion Magnet Insulation	326,250
Physical Model Development and Benchmarking for MHD Flows in Blanket Design	326,250
Novel, High Energy Density Intermetallic Anode Material for Li-Ion Batteries	375,000
Self-Cleaning Surfaces with Morphology Mimicking Superhydrophobic Biological Surfaces	374,985
Investigation of $(CaO)_x(Al_2O_3)_x$ for Thermal Insulation and Molten Aluminum Contact	374,449
FY 2005 PHASE II (SECOND YEAR)	$6,117,197
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
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
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$14,886,071
FY 2005 PHASE I	$4,584,326
Rapid Microfluidic Production of Multiple PET Biomarkers	99,638
Universal Probe Reagents for Detection and Quantitation of RNA Splicing	99,071
Membrane Nano-fragment Preparation Technology	99,988
Cost Effective Ulta-Thin Palladium Based Membrane for Hydrogen Separation and Purification	99,998
Novel Polycarbonate Synthesis Using Carbon Dioxide as a Feedstock	99,924
Novel Sorbents for Air Separation	100,000
Low-Cost High-Temperature Heat Exchanger for Solid Oxide Fuel Cells using a Near-Net-Shape Ceramic Powder Forming Process	97,715
Maintainable Solution-Derived Nanocoatings for Advanced Boiler Systems	99,996
Development of Electrically Mediated Electrophoretic Deposition for Thermal Barrier Coating Systems	100,000
High Performance Electrolytes for Electrochemical Capacitors	100,000
Low Cost Synthesis of High Surface Area Thermally Stable Lithium-Ion Battery	99,993
Electrolytic Process to Produce Sodium Hypochlorite Using NaSICON Ceramic Membranes	99,860
Novel Supported Carbon-Silica Nanocomposite Membranes for Air Separation	100,000

OFFICE OF SCIENCE (continued)

OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)

TECHNOLOGY RESEARCH DIVISION (continued)

SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)

FY 2005 PHASE I (continued)

	FY 2005
Hybrid Anti-Fouling Membrane System for Natural Gas Separation	100,000
Hybrid Membrane Distillation Process for Enhanced Integrated Ethanol Production	100,000
Nanocomposite Catalytic Membrane for Reagentless Hydrogen Peroxide Production	99,998
High Stability Thin Film Composite Reverse Osmosis Membranes	99,997
Novel Nanoporous Polymer Membranes for Gas and Vapor Separation	100,000
Enhanced Catalysts from Nanostructured Materials	97,981
Multimodal Acoustic Mixing Process for Carbon Nanotube Polymer Composites	100,000
Nanostrucutred Catalysts for Olefin Conversion	100,000
New Synthesis Route to Styrene Using Designer Ionic Liquids	99,993
A Novel Growth Technique for Large Diameter AlN Single Crystal	99,582
Systems-Based Design of Ferritic-Martensitic Superalloys for Generation IV Nuclear Reactors	99,910
Inorganic/Organic Flexible Nanocomposites with High Thermoelectric Figure of Merit	99,979
An Advanced Nanophosphor Technology for General Illumination	99,979
Abrasion-Resistant Membranes for Biomass Hydrolysate Clarification	100,000
Dimensionally Stable High Performance Membrane	99,929
Nano-Fabricated Hydrogen Separation Membranes	99,799
Low Cost Carbon Fiber Composites for Lightweight Vehicle Parts	100,000
Manufacturing Process for Novel Solid State Lighting Phosphors	99,997
Development of Low Cost Manufacturable Shape Memory Foams for Automotive Shock Energy Adsorption	99,899
Metal Hydride Slurry as a Novel Carrier of Hydrogen	99,003
Boron Nitride Capacitors for Advanced Power Electronic Devices	100,000
Improved Internal-Tin Nb3Sn Conductors for ITER and Other Fusion Applications	99,503
Flow Channel Inserts for Dual-Coolant ITER Test Blanket Modules	99,991
Inert-Gas Buffering for Particle Size Separation of Superconductor Precursor Powders	100,000
New Highly Radiation-Resistant Insulation Process for High Field Accelerator Magnets	99,990
Internal-Tin Nb/Sn Strand with Enhanced Ti Additions Aimed at 17 T Optimization	100,000
Development of MgB_2 for Near Term HEP Applications	100,000
Feasibility of Cost-Effective, Long Length, BSCCO 2212 Round Wires, for Very High Field Magnets Beyond 12 Tesla at 4.2 Kelvin	99,793
An Advanced Ternary Nb_3Sn with ZrO_2 Precipitates Via the PIT Process	100,000
Composite Filament, Nb_3Sn Superconductor for HEP Applications	99,993
A New PIT Nb_3Sn Process, Toward Improved Cost-Performance for HEP High Field Magnets	99,540
Microwave Joining of Ceramic Structures for Advanced High Energy Accelerators Using a Novel Quasi-Optical Elliptical Cavity	99,866
Commercial and Cost Effective Production of Gas Electron Multiplier (GEM) Foils	99,465
Production Crystal Growth System Design for Aluminum Antimonide (AlSb)	93,880

OFFICE OF SCIENCE (continued)

	FY 2005
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
TECHNOLOGY RESEARCH DIVISION (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING (continued)	
FY 2005 PHASE II (FIRST YEAR)	$3,949,453
Engineered Surfaces for the Lithium Tokamak Experiment	325,000
Moldable Ceramic Composites for High Field Magnet Applications	174,913
Low Loss Ferroelectric Material Development for Accelerator Applications	325,000
Advanced Fluoropolymer Vessels for Ultra-Clean Ionization and Scintillation Detectors	325,000
Coaxial Energetic Ion Depostition of Superconducting Coatings on Copper RF Cavities for Particle Accelerators	350,000
A Method for Electroforming Copper with Ultra-Low Levels of Radioactivity	350,000
Polythiophosphonate Electrolytes for Rechargeable Magnesium Batteries	374,835
Lithium Ion-Channel Polymer Electrolyte for Lithium Metal Anode Rechargeable Batteries	375,000
High Efficiency Nanocomposite White Light Phosphors	374,707
Functionally Graded Aluminum Nitride - Oxide Coatings for Hot Pipe Protection	374,998
Development of Solar Grade (SoG) Silicon	300,000
An Innovative Technique of Preparing Solar Grade Silicon Wafers from Metallurgical Grade Silicon by In-Situ Purification	300,000
FY 2005 PHASE II (SECOND YEAR)	$6,352,292
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

OFFICE OF SCIENCE (continued)

	FY 2005
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
TECHNOLOGY RESEARCH DIVISION (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES	$9,293,851
FY 2005 PHASE I	$1,297,663
Reliable High Performance Carbon Nanotube and LaB_6 Nanowire Field Emission Cathodes for STEM	100,000
A Silicon Carbide Switch for High Energy Physics Applications	99,400
Novel Solid State Photodetector to Enable Future Scintillating Fiber Detection Experiments	100,000
UV-Sensitive Solid State Photodetector for Dark Matter Detection Using Liquid Xenon	100,000
High Temperature, Superconducting, Thinfilm Coatings for RF Accelerator Cavities	100,000
SQUID-based Nondestructive Testing Equipment of Dished Niobium Sheets for SRF Cavities	99,996
Improved Nb For Superconducting RF Cavities	99,245
High Z Droplets -- A Novel Source of Heavy Ions for Nuclear Physics	99,967
Germanium-76 Isotope Separation by Cryogenic Distillation	99,933
Three-Dimensional High-Resolution Gamma Ray Detector for RIA	100,000
Segmentation of the Outer Contact on P-Type Coaxial Germanium Detectors	99,840
Fast, Dense, Low Cost Scintillator for Nuclear Physics	100,000
Combinatorial Approach for the Discovery of New Scintillating Materials	99,282
FY 2005 PHASE II (FIRST YEAR)	$724,995
Novel Scintillator for Nuclear Physics Studies	350,000
Ultra-Sensitive, Compact Mid-Infrared Spectrometer for Airborne and Ground-Based Atmospheric Monitoring	374,995
FY 2004 PHASE II (SECOND YEAR)	$7,271,193
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

OFFICE OF SCIENCE (continued)

	FY 2005
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
TECHNOLOGY RESEARCH DIVISION (continued)	
SMALL BUSINESS INNOVATION RESEARCH PROGRAM (continued)	
INSTRUMENTATION AND FACILITIES (continued)	
FY 2004 PHASE II (SECOND YEAR) (continued)	
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
MATERIALS STRUCTURE AND COMPOSITION	$912,489
FY 2005 PHASE I	$199,989
Nano Graphene Plate-Reinforced Polymer Composites	100,000
Advanced Tungsten Structures for Plasma-Facing Components in Magnetic Confinement Fusion Energy Reactors	99,989
FY 2005 PHASE II (FIRST YEAR)	$712,500
Microstructural Refinement of Tantalum for Superconductor Diffusion Barrier Applications	337,500
"Metal Rubber" Nanostructured Materials	375,000
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM	$2,420,858
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$871,869
FY 2005 PHASE I	$199,898
An Advanced Power Converter System Using High Temperature, High Power Density SiC Devices	99,898
Economical High Performance Thermoplastic Composite Bipolar Plates	100,000
FY 2005 PHASE II (FIRST YEAR)	$296,971
A Compact, In-Situ Instrument for Organic Acid Areosols	296,971
FY 2005 PHASE II (SECOND YEAR)	$375,000
Engineered Tungsten Surfaces for IFE Dry Chamber Walls	375,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$99,818
FY 2005 PHASE I	$99,818
Property Measurement and Improved Strength of Duplex SiC/SiC Ceramic Composites for Fast Reactor Fuel Cladding	99,818

OFFICE OF SCIENCE (continued)

	FY 2005
OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH (continued)	
TECHNOLOGY RESEARCH DIVISION (continued)	
SMALL BUSINESS TECHNOLOGY TRANSFER PROGRAM (continued)	
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$1,049,171
FY 2005 PHASE I	$299,225
Ultra-high Productivity Metal Membranes for Hydrogen Production Applications	99,533
Development of Low Cost Conducting Polymer for Electrostatic Precipitators	99,704
High-Energy-Density Nanocomposite Nd-Fe-B/Fe Magnets for Advanced Generator/ Motor Applications	99,988
FY 2005 PHASE II (SECOND YEAR)	$749,946
Nanostructured Polymeric Heterogeneous Catalyst for Industrial Applications	375,000
Novel Approach Toward High Performance Energetic Rays Detection	374,946
INSTRUMENTATION AND FACILITIES	$400,000
FY 2005 PHASE I	$100,000
Reverse Emittance Exchange for Muon Colliders	100,000
FY 2005 PHASE II (FIRST YEAR)	$300,000
High Brightness Neutron Source for Radiography	300,000
OFFICE OF FUSION ENERGY SCIENCES	$8,600,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$8,600,000
Vanadium Alloy and Insulating Coating Research	900,000
Theory and Modeling	1,900,000
Ferritic/Martensitic Steel Research	2,200,000
SiC/SiC Composites Research	1,600,000
Plasma Facing Materials Research	2,000,000
OFFICE OF BIOLOGICAL & ENVIRONMENTAL RESEARCH	$1,199,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$1,199,000
Physical, Chemical and Structural Evolution of Zeolite-containing Waste Forms Produced from Metakaolinite and Calcined HLW	205,000
Investigating Ultrasonic Diffraction Grating Spectroscopy and Reflection Techniques for Characterizing Slurry Properties	268,000
Chemistry of Actinides in Molten Glasses and its Correlation to Structural Performance of Solid Glasses: Filling the Knowledge Gap	136,000
Stability of High Level Radioactive Waste Forms	330,000
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 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 the active 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 Condensed Matter Theory activity supports basic research in theory, modeling, and simulations complementing the experimental effort. A current major thrust is in nanoscale science where links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are poorly understood. Other research areas include correlated behavior of two dimensional electron gases, quantum transport, superconductivity, magnetism, and optics. An important facilitating component is the Computational Materials Science Network (CMSN) which enables groups of scientists from Department of Energy (DOE) national laboratories, universities, and (to a lesser extent) industry to address materials problems requiring larger-scale collaboration across disciplinary and organizational boundaries. The FY 2005 funding for this program is $19,798,000 and the DOE contact is Dale D. Koelling, (301) 903-2187.

EXPERIMENTAL CONDENSED MATTER PHYSICS

This program supports activities in experimental condensed matter physics that emphasize the relationship between electronic structure and the properties of complex systems whose behavior is often derived from electron correlation. Major efforts are in systems that exhibit correlated and emergent behavior with superconducting, semiconducting, magnetic, thermoelectric, and optical properties. These efforts are accompanied by activities to synthesize and characterize single crystals to further explore and discover new and novel correlated electron behavior. The program supports the development of new techniques and instruments for characterizing the properties of these materials under extreme conditions of ultra low temperature (mK) and ultra high magnetic fields (100 T). One main emphasis of this activity is on the electron dynamics of low dimensional systems. Confinement effects in high purity semiconductors produce new forms of matter and new physical phenomena such as the fractional Quantum Hall effect and Bose-Einstein Condensates. These low dimensional systems and other nanophase materials offer rich opportunities to explore their novel electronic behaviors. In addition, this activity seeks to exploit ultrafast tools to manipulate and probe the dynamic electronic behavior of condensed matter through the development and applications of laser-driven, table-top x-ray sources. The FY 2005 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 supports basic research in the design and synthesis of novel materials and material constructs with an emphasis on the chemistry and chemical control of structure and collective properties. Major thrust areas include: 1) nanoscale chemical synthesis and assembly - synthesis of nanoscale materials, manipulation of their properties, and organization of nanoscale materials into macroscopic structures; 2) solid state chemistry - exploratory synthesis and discovery of new classes of electrical conductors and superconductors, magnets, thermoelectric and ferroelectric materials, and porous materials with controlled porosities and tailored reactivities; 3) polymers - exploring and exploiting the self-assembly of block copolymers, polymer composites, and polymers with novel electronic and optical properties; 4) surface and interfacial chemistry - electrochemistry, electro-catalysis, friction, adhesion and lubrication at the nanoscale, and development of new, science-driven, laboratory-based analytical tools and techniques; and 5) biomolecular materials - biomimetic/bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology. The FY 2005 funding for this program is $46,860,000 and the DOE contacts are Richard Kelley, (301) 903-6051 and Aravinda Kini (301) 903-3565.

MECHANICAL BEHAVIOR AND RADIATION EFFECTS

This activity supports basic research to understand the deformation, embrittlement, fracture, and radiation damage of materials with an emphasis on the relationships between mechanical behavior and radiation effects and defects in the material. This research builds on atomic level understanding of the relationship between mechanical behavior and defects in order to develop predictive models of materials behavior for the design of materials having superior mechanical behavior such as at very high temperatures. The mechanical behavior of materials under repeated or cyclic stress, high rates of stress application, and over a range of temperatures and stress conditions are relevant to present and projected energy conversion systems. The focus on radiation effects is to achieve atomic level understanding of radiation damage mechanisms and subsequent materials property changes to design radiation-tolerant materials for advanced energy systems. Important radiation induced materials property changes include embrittlement, stress-corrosion cracking, amorphization (transition from a crystalline to a non-crystalline phase), and ion irradiation-induced surface modification. The FY 2005 funding for this program is

$14,008,000 and the DOE contact is Yok Chen, (301) 903-4174.

X-RAY AND NEUTRON SCATTERING

This activity supports basic research in condensed matter physics and materials physics using neutron and x-ray scattering capabilities, primarily at major BES-supported user facilities. Research seeks to achieve a fundamental understanding of the atomic, electronic, and magnetic structures and excitations of materials as well as the relationship of these structures and excitations to the physical properties of materials. The continuing development and improvement of next-generation instrumentation including a full range of elastic, inelastic, and imaging techniques as well as ancillary technologies such as novel detectors, sample environment, data analysis, and technology for producing polarized neutrons is also supported. The FY 2005 funding for this program is $46,061,000 and the DOE contact is Helen Kerch, (301) 903-2346.

STRUCTURE AND COMPOSITION OF MATERIALS

This activity supports basic research in condensed matter physics and materials physics using electron scattering and microscopy and scanning probe techniques. Research includes experiments and theory to understand the atomic, electronic, and magnetic structures of materials. Increasingly important are the nanoscale structures and the structure and composition of inhomogeneities including defects, interfaces, surfaces, and precipitates. Advancing the state of the art of electron beam and scanning probe techniques and instrumentation for quantitative microscopy and microanalysis is an essential element in this portfolio. The FY 2005 funding for this program is $24,907,000 and the DOE contact is Jane Zhu, (301) 903-3811.

PHYSICAL BEHAVIOR

This activity is a fundamental research program focusing on the functional properties of materials. The major emphasis is on the behavior of complex materials in response to external stimuli often encountered in energy-intensive applications. This basic research program focuses on physical responses (such as optical, electronic, or magnetic changes) to temperature, electro-magnetic fields, chemical environments, and the proximity effects of surfaces and interfaces with an emphasis on the relationships between physical behavior and the microstructure and defects in the material. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the semiconducting, superconducting and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures in energy conversion processes; and diffusion and transport phenomena in ceramic electrolytes for improved performance in batteries and fuel cells. Basic research is also supported to develop new instrumentation, including in-situ experimental tools, to probe the physical behavior in real environments encountered in energy applications. The FY2005 funding for this program is $25,551,000 and the DOE contact is Refik Kortan, (301) 903-3308.

SYNTHESIS AND PROCESSING SCIENCES

This activity supports basic research in synthesis and processing science for innovative synthesis of new materials with desired structure, properties or behavior; to understand the physical phenomena which underpin materials synthesis such as diffusion, nucleation and phase transitions; and to develop in situ monitoring and diagnostic capabilities. Examples of activities in synthesis and processing include: (1) the physics of growth of complex thin films and nanoscale objects with an emphasis on atomic layer-by-layer control; (2) preparation techniques for novel single crystal and bulk materials having novel nanoscale attributes; (3) understanding the contributions of the liquid and other precursor states to the processing of bulk nanoscale materials; and (4) low energy processing techniques for large scale nanostructured materials. This activity includes the operation of the Materials Preparation Center at the Ames Laboratory, which develops innovative and superior processes for materials preparation and provides small quantities of research grade, controlled purity materials and crystals that are otherwise not available to academic, governmental, and industrial research communities for research purposes. The FY 2005 funding for this program is $15,149,000 and the DOE contact is Timothy Fitzsimmons, (301) 903-9830.

ENGINEERING PHYSICS

Engineering Research advances scientific understanding underlying the dynamic interactions of single and multicomponent solid and fluid systems. Research considers the behavior and interactions of fluids including organic, biological, and complex fluids with each other and with solid systems; the transport of energy on and within these systems; and the development of means to advance the characterization of these systems. Issues under consideration frequently span several orders of magnitude in length and time scales and range from atomic interactions to macroscopic behavior and subpicosecond chemical events to fatigue events that may take years to reach completion. Accordingly they present a considerable challenge to theory, computational simulation, and experiment. Questions of interest have included understanding and predicting the behavior of: 1) nanoscale structures and systems, including those with biological components; 2) dynamics of fluids, especially multi-component and complex fluids, but also including heat transfer, solidification, and granular materials; and 3) interactions of phonons with interfaces, secondary phases, or micro- and nanoscale defects in solids. The FY 2005 funding for this program is $5,306,000 and the DOE contact is Tim Fitzsimmons, (301) 903-9830.

EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH

The Department of Energy (DOE) Experimental Program to Stimulate Competitive Research (EPSCoR) activity supports basic research spanning the broad range of science and technology programs within DOE in states that have historically received relatively less federal research funding. EPSCoR includes the states of Alabama, Alaska, Arkansas, Delaware, Hawaii, Idaho, Kansas, Kentucky, Louisiana, Maine, Mississippi, Montana, Nebraska, Nevada, New Hampshire, New Mexico, North Dakota, Oklahoma, Rhode Island, South Carolina, South Dakota, Tennessee, Vermont, West Virginia, and Wyoming, as well as the Commonwealth of Puerto Rico and the U.S. Virgin Islands. BES manages EPSCoR for the Department. The FY 2005 funding for the materials component of this program is $7,643,000 and the DOE contact is Arvinda Kini, (301) 903-3565.

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 next generation short-pulse spallation neutron source that will be significantly more powerful than the best spallation neutron source now in existence—ISIS at the Rutherford Laboratory in England. On the drawing board is the Linac Coherent Light Source (LCLS) at Stanford Linear Accelerator Center, which is a free-electron laser that will provide laser-like radiation in the X-ray region of the spectrum that is 10 orders of magnitude greater in peak power and peak brightness than any existing coherent Xray light source. The FY 2005 funding for this program is $326,326,000 and the DOE contact is Pedro A. Montano, (301) 903-2347.

NANOSCIENCE CENTERS

This activity supports construction and the subsequent operation of Nanoscale Science Research Centers (NSRCs) at DOE laboratories that already host one or more of the BES major user facilities. Nanotechnology is the creation and use of materials, devices, and systems through the control of matter at the nanometer-length scale, at the level of atoms, molecules, and supramolecular structures. Nanoscience and nanotechnology will fundamentally change the way materials and devices will be produced in the future and subsequently revolutionize the production of virtually every human-made object. Nanoscience will explore and develop the rules and tools needed to fully exploit the benefits of nanotechnology. Each NSRC will combine state-of-the-art equipment for materials nanofabrication with advanced tools for nano characterization. The NSRCs will become a cornerstone of the Nation’s nanotechnology revolution, covering the full spectrum of nano-materials and providing an invaluable resource for universities and industries. The FY 2005 funding for this program is $112,460,000 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

SMALL BUSINESS INNOVATION RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2005 PHASE I

Very High Temperature (400+ C), High Power Density Silicon Carbide (SiC) Power Electronic Converters - DOE Contact Imre Gyuk, (202) 586-1482; Arkansas Power Electronics International, Inc. Contact Sharmila D. Mounce, (479) 443-5759

Universal Converter Using Silicon Carbide - DOE Contact Imre Gyuk, (202) 586-1482; Peregrine Power, LLC Contact Mr. Dallas Austin Marckx, (503) 682-7001

A New Scintillator for Time-of-Flight PET - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 668-6800

High Efficiency, Low Cost Scintillators for PET - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 668-6800

A Very High Spatial Resolution Detector for Small Animal PET - DOE Contact Peter Kirchner, (301) 903-9106; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 668-6800

High-Temperature Ceramic Capacitors for Applications in Deep Drilling and Completion Processes - DOE Contact Tony Zammerilli, (304) 285-4641; Synergistic Advanced Technologies, LLC Contact Thomas L. Venable, (520) 760-0291

Abuse Tolerant, Voltage Stabilized Li-ion Cell - DOE Contact Jim Barnes, (202) 586-5657; Farasis Energy, Inc. Contact Dr. Keith Douglas Kepler, (510) 732-6600

Organic Additives as Redox Shuttles for Overcharge Protection of Lithium Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Lithium Power Technologies, Inc. Contact Dr. Mohammed Z. Munshi, (281) 489-4889

Improved Low-Temperature Performance of Safer, Low-Cost Lithium Iron Phosphate Cathodes for Lithium-Ion Batteries - DOE Contact Jim Barnes, (202) 586-5657; Tiax, LLC Contact Renee Wong, (617) 498-5655

Safer, Non-Toxic, Alternative Electrolytes - DOE Contact Jim Barnes, (202) 586-5657; Toxco Inc. Contact James J. Gormley, (610) 522-5960

Novel Large Area High Resolution Neutron Detector for the Spallation Neutron Source - DOE Contact Helen Kerch, (301) 903-2346; Proportional Technologies, Inc. Contact Dr. Jeffrey L. Lacy, (713) 747-7324

Extreme Environment Control Sensors - DOE Contact Madeline Feltus, (301) 903-2308; Luna Innovations Incorporated Contact Wendy Vogt, (540) 552-5128

Refractory Substrate/Capillary Assisted/Thin Flowing Lithium Film Plasma Facing Component - DOE Contact Gene Nardella, (301) 903-4956; Advanced Cooling Technologies, Inc. Contact Dr. Jon Zuo, (717) 295-6058

Innovative Nanoparticle Insulation Systems for Fusion Magnets - DOE Contact Warren Marton, (301) 903-4936; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Modified Epoxy Resin Systems as Composite Insulation in Fusion Confinement Systems - DOE Contact Warren Marton, (301) 903-4936; Eltron Research Inc. Contact Eileen E. Sammells, (303) 530-0263

Fabrication of Complex Copper Cooling Devices Using Ultrasonic Metal Consolidation to Locally Cool and Monitor High Energy Electron Sources - DOE Contact L.K. Len, (301) 903-3233; Solidica, Inc. Contact Dr. Dawn R. White, (734) 222-4680

Cost-Effective, High-Performance, High-Purity Niobium Superconducting Radio Frequency Cavities - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Ultramet Contact Craig N. Ward, (818) 899-0236

FY 2005 PHASE II (FIRST YEAR)

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

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

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

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

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

High Efficiency, White TOLED Devices for Lighting Applications - DOE Contact James Brodrick, (202) 586-1856; Universal Display Corporation Contact 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 Roger Buelow, (440) 836-7421

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

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

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

FY 2005 PHASE II (SECOND 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 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 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 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 Dan Wittkopp, (360) 378-4137

New N+ Contact for Germanium Strip Detectors - DOE Contact Manouchehr Farkhondeh, (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 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 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 John A. Rice, (303) 684-9242

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2005 PHASE I

High Throughput Microcantilever-Based Detection of Antigen-Antibody Binding - DOE Contact Marvin Stodolsky, (301) 903 4475; Femtogen Contact Dr. David Altman, (503) 750-6501

Evaluation of Nuclear Grade SiC/SiC Composites for Control Rod Sheaths - DOE Contact Sue Lesica, (301) 903-8755; Hyper-therm High-temperature Composites, Inc. Contact Wayne S. Steffier, (714) 375-4085

Nanotechnology Enabled Advanced Industrial Heat Transfer Fluids - DOE Contact Bob Gemmer, (202) 586-5885; Nei Corporation Contact Dr. Ganesh Skandan, (732) 868-1906

Micro/Nano-Encapsulation of Partial Oxidation Biocatalysts - DOE Contact Charlie Russomanno, (202) 586-7543; Lnkchemsolutions Contact Dr. Gustavo F. Larsen, (402) 416-1811

Improvement of the Properties of Tubular Internal-Tin Nb_3Sn - DOE Contact L.K. Len, (301) 903-3233; Supergenics I, LLC Contact Bruce A. Zeitlin, (941) 544-8795

FY 2005 PHASE II (FIRST YEAR)

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

Physical Model Development and Benchmarking for MHD Flows in Blanket Design - DOE Contact Gene Nardella, (301) 903-4956; Hypercomp, Inc. Contact Dr. Vijaya Shankar, (818) 865-3713

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

FY 2005 PHASE II (SECOND 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 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 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 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 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 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 Sharon Fehrenbacher, (410) 224-3710

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

High Pressure Economical Process for Treating Natural Gas - DOE Contact Tony Zammerilli, (304) 285-4641; TDA Research, Inc. Contact 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 Manouchehr Farkhondeh, (301) 903-4398; Sienna Technologies, Inc. Contact Dr. Ender Savrun, (425) 485-7272

A Novel Design for CZT Gamma Ray Spectrometers - DOE Contact Manouchehr Farkhondeh, (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 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

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2005 PHASE I

Rapid Microfluidic Production of Multiple PET Biomarkers - DOE Contact Prem Srivastava, (301) 903-4071; Nanotek, LLC Contact Debbie M. Matteo, (865) 980-1916

Universal Probe Reagents for Detection and Quantitation of RNA Splicing - DOE Contact Marvin Stodolsky, (301) 903-4475; Callida Genomics Inc. Contact Dr. Radoje Drmanac, (408) 739-2353

Membrane Nano-fragment Preparation Technology - DOE Contact Marvin Stodolsky, (301) 903-4475; Physical Optics Corporation Contact Gordon E. Drew, (310) 320-3088

Cost Effective Ulta-Thin Palladium Based Membrane for Hydrogen Separation and Purification - DOE Contact Jose Figueroa, (412) 386-4966; Innovatek, Inc. Contact Dr. Patricia M. Irving, (509) 375-1093

Novel Polycarbonate Synthesis Using Carbon Dioxide as a Feedstock - DOE Contact David Lang, (412) 386-4881; Novomer LLC Contact Tony Eisenhut, (607) 257-6830

Novel Sorbents for Air Separation - DOE Contact Jenny Tennant, (304) 285-4830; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

Low-Cost High-Temperature Heat Exchanger for Solid Oxide Fuel Cells using a Near-Net-Shape Ceramic Powder Forming Process - DOE Contact Magda Rivera, (304) 285-1359; Spinworks LLC Contact James Daniel Briselden, (814) 899-4871

Maintainable Solution-Derived Nanocoatings for Advanced Boiler Systems - DOE Contact Udaya Rao, (412) 386-4743; Applied Thin Films, Inc. Contact John Rechner, (847) 467-5235

Development of Electrically Mediated Electrophoretic Deposition for Thermal Barrier Coating Systems - DOE Contact Charles T. Alsup, (304) 285-5432; Faraday Technology, Inc. Contact Dr. E. Jennings Taylor, (937) 836-7749

High Performance Electrolytes for Electrochemical Capacitors - DOE Contact Jim Barnes, (202) 586-5657; ADA Technologies, Inc. Contact Clifton H. Brown. Jr., (303) 792-5615

Low Cost Synthesis of High Surface Area Thermally Stable Lithium-Ion Battery - DOE Contact Jim Barnes, (202) 586-5657; Eltron Research Inc. Contact Eileen E. Sammells, (303) 530-0263

Electrolytic Process to Produce Sodium Hypochlorite Using NaSICON Ceramic Membranes - DOE Contact Charlie Russomanno, (202) 586-7543; Ceramatec, Inc. Contact Raymond K. Miller, (801) 978-2114

Novel Supported Carbon-Silica Nanocomposite Membranes for Air Separation - DOE Contact Charlie Russomanno, (202) 586-7543; Ceramem Corporation Contact Dr. Richard J. Higgins, (781) 899-4495

Hybrid Anti-Fouling Membrane System for Natural Gas Separation - DOE Contact Charlie Russomanno, (202) 586-7543; Compact Membrane Systems, Inc. Contact Dr. Stuart M. Nemser, (302) 999-7996

Hybrid Membrane Distillation Process for Enhanced Integrated Ethanol Production - DOE Contact Charlie Russomanno, (202) 586-7543; Compact Membrane Systems, Inc. Contact Stuart M. Nemser, (302) 999-7996

Nanocomposite Catalytic Membrane for Reagentless Hydrogen Peroxide Production - DOE Contact Charlie Russomanno, (202)586-7543; Eltron Research Inc. Contact Eileen E. Sammells, (303) 530-0263

High Stability Thin Film Composite Reverse Osmosis Membranes - DOE Contact Charlie Russomanno, (202) 586-7543; Eltron Research Inc. Contact Eileen E. Sammells, (303) 530-0263

Novel Nanoporous Polymer Membranes for Gas and Vapor Separation - DOE Contact Charlie Russomanno, (202) 586-7543; Membrane Technology And Research, Inc. (MTR) Contact Elizabeth G. Weiss, (650) 328-2228

Enhanced Catalysts from Nanostructured Materials - DOE Contact Charlie Russomanno, (202) 586-7543; Lynntech, Inc. Contact Dr. G. Duncan Hitchens, (979) 693-0017

Multimodal Acoustic Mixing Process for Carbon Nanotube Polymer Composites - DOE Contact Charlie Russomanno, (202) 586-7543; Resodyn Corporation Contact Lawrence C. Farrar, (406) 497-5252

Nanostrucutred Catalysts for Olefin Conversion - DOE Contact Charlie Russomanno, (202) 586-7543; TDA Research, Inc. Contact John D. Wright, (303) 940-2300

New Synthesis Route to Styrene Using Designer Ionic Liquids - DOE Contact Charlie Russomanno, (202) 586-7543; Exelus, Inc. Contact Mitrajit Mukherjee, (973) 740-2350

A Novel Growth Technique for Large Diameter AlN Single Crystal - DOE Contact James Brodrick, (202) 586-1856; Fairfield Crystal Technology, LLC Contact Andrew G. Timmerman, (860) 354-2111

Systems-Based Design of Ferritic-Martensitic Superalloys for Generation IV Nuclear Reactors - DOE Contact Sue Lesica, (301) 903-8755; Questek Innovations, LLC Contact Raymond P. Genellie, Jr., (847) 425-8211

Inorganic/Organic Flexible Nanocomposites with High Thermoelectric Figure of Merit - DOE Contact Kevin Stork, (202) 586-8306; Aspen Systems Inc. Contact Dr. Kang P. Lee, (508) 481-5058

An Advanced Nanophosphor Technology for General Illumination - DOE Contact James Brodrick, (202) 586-1856; Boston Applied Technologies, Inc. Contact Dr. Yingyin Kevin Zou, (781) 935-2800

Abrasion-Resistant Membranes for Biomass Hydrolysate Clarification - DOE Contact Richard Orrison, (202) 586-1633; Ceramem Corporation Contact Dr. Richard Higgins, (781) 899-4495

Dimensionally Stable High Performance Membrane - DOE Contact Donna Ho, (202) 586-8000; Giner, Inc. Contact Dr. Anthony B. LaConti, (781) 529-0501

Nano-Fabricated Hydrogen Separation Membranes - DOE Contact Charlie Russomanno, (202) 586-7543; ITN Energy Systems, Inc. Contact Janet Casteel, (303) 285-5111

Low Cost Carbon Fiber Composites for Lightweight Vehicle Parts - DOE Contact Richard Orrison, (202) 586-1633; Material Innovation Technology, Llc Contact James E. Stike, (828) 674-5517

Manufacturing Process for Novel Solid State Lighting Phosphors - DOE Contact James Brodrick, (202) 586-1856; Phosphortech Corporation Contact Dr. Christopher J. Summers, (404) 664-5008

Development of Low Cost Manufacturable Shape Memory Foams for Automotive Shock Energy Adsorption - DOE Contact Richard Orrison, (202) 586-1633; Shape Change Technologies Contact Dr. Andrew Peter Jardine, (805) 497-2549

Metal Hydride Slurry as a Novel Carrier of Hydrogen - DOE Contact Matthew Kauffman, (202) 586-5824; Tiax, LLC Contact Renee Wong, (617) 498-5655

Boron Nitride Capacitors for Advanced Power Electronic Devices - DOE Contact Jim Ahlgrimm, (202) 586-9806; Integrated Micro Sensors, Inc. Contact Dr. David Starikov

Improved Internal-Tin Nb_3Sn Conductors for ITER and Other Fusion Applications - DOE Contact Warren Marton, (301) 903-4936; Supergenics I, LLC Contact Bruce A. Zeitlin, (941) 544-8795

Flow Channel Inserts for Dual-Coolant ITER Test Blanket Modules - DOE Contact Gene Nardella, (301) 903-4956; Ultramet Contact Craig N. Ward, (818) 899-0236

Inert-Gas Buffering for Particle Size Separation of Superconductor Precursor Powders - DOE Contact L.K. Len, (301) 903-3233; Accelerator Technology Corporation Contact Dr. Peter M. McIntyre, (979) 255-5531

New Highly Radiation-Resistant Insulation Process for High Field Accelerator Magnets - DOE Contact L.K. Len, (301) 903-3233; Composite Technology Development, Inc. Contact Dr. Naseem A. Munshi, (303) 664-0394

Internal-Tin Nb/Sn Strand with Enhanced Ti Additions Aimed at 17 T Optimization - DOE Contact L.K. Len, (301) 903-3233; Global Research and Development, Inc. Contact Michael Tomsic, (937) 332-0348

Development of MgB_2 for Near Term HEP Applications - DOE Contact L.K. Len, (301) 903-3233; Hyper Tech Research, Inc. Contact Michael Tomsic, ((937) 332-0348

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; Sci Engineered Materials, Inc. Contact Daniel Rooney, (614) 486-0261

An Advanced Ternary Nb_3Sn with ZrO_2 Precipitates Via the PIT Process - DOE Contact L.K. Len, (301) 903-3233; Supercon, Inc. Contact Terence Wong, (508) 842-0174

Composite Filament, Nb_3Sn Superconductor for HEP Applications - DOE Contact L.K. Len, (301) 903-3233; Superconducting Systems, Inc. Contact Dr. Shahin Pourrahimi, (781) 642-6702

A New PIT Nb_3Sn Process, Toward Improved Cost-Performance for HEP High Field Magnets - DOE Contact L.K. Len, (301) 903-3233; Supramagnetics, Inc. Contact Dr. Leszek Richard Motowidlo, (860) 977-7416

Microwave Joining of Ceramic Structures for Advanced High Energy Accelerators Using a Novel Quasi-Optical Elliptical Cavity - DOE Contact L.K. Len, (301) 903-3233; Rwbruce Associates, Inc. Contact Dr. Ralph W. Bruce, (443) 822-3605

Commercial and Cost Effective Production of Gas Electron Multiplier (GEM) Foils - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Tech-Etch, Inc. Contact George E. Keeler, (508) 747-0300

Production Crystal Growth System Design for Aluminum Antimonide (AlSb) - DOE Contact Frances Keel, (202) 586-8329; ALSB Crystal Technology, Inc. Contact Dr. John W. Sherohman, (925) 449-0761

FY 2005 PHASE II (FIRST YEAR)

Engineered Surfaces for the Lithium Tokamak Experiment - DOE Contact Gene Nardella, (301) 903-4956; Plasma Processes, Inc. Contact Timothy N. McKechnie, (256) 851-7653

Moldable Ceramic Composites for High Field Magnet Applications - DOE Contact L.K. Len, (301) 903-3233; Multiphase Composites Contact 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 Andrew K. MacIntyre, (401) 253-0200

Coaxial Energetic Ion Depostition of Superconducting Coatings on Copper RF Cavities for Particle Accelerators - DOE Contact Manouchehr Farkhondeh, (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 Manouchehr Farkhondeh, (301) 903-4398; Reeves & Sons, LLC Contact James H. Reeves, (509) 943-1653

Polythiophosphonate Electrolytes for Rechargeable Magnesium Batteries - DOE Contact Jim Barnes, (202) 586-5657; Phoenix Innovation Inc. Contact 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 John D. Wright, (303) 940-2300

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

Functionally Graded Aluminum Nitride - Oxide Coatings for Hot Pipe Protection - DOE Contact Sara Dillich, (202) 586-7925; Eltron Research, Inc. Contact 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 Jonathan A. Talbott, (603) 883-5200

FY 2005 PHASE II (SECOND 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 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 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 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 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 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 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 Elizabeth Weiss, (650) 328-2228

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

Nanocomposite Dielectric Materials for High Frequency Applications - DOE Contact T. V. George, (301) 903-4957; TPL, Inc. Contact 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

INSTRUMENTATION AND FACILITIES

FY 2005 PHASE I

Reliable High Performance Carbon Nanotube and LaB_6 Nanowire Field Emission Cathodes for STEM - DOE Contact Dean Miller, (630) 252-4108; Xintek, Inc. Contact Dr. Shan Bai, (919) 524-4702

A Silicon Carbide Switch for High Energy Physics Applications - DOE Contact L.K. Len, (301) 903-3233; Mount Blodgett Design, Inc. Contact Robert J. Callanan, (719) 598-0381

Novel Solid State Photodetector to Enable Future Scintillating Fiber Detection Experiments - DOE Contact Saul Gonzalez, (301) 903-2359; Amplification Technologies, Inc. Contact Dr. Alexander Krutov, (646) 361-3255

UV-Sensitive Solid State Photodetector for Dark Matter Detection Using Liquid Xenon - DOE Contact Saul Gonzalez, (301) 903-2359; Amplification Technologies, Inc. Contact Dr. Alexander Krutov, (646) 361-3255

High Temperature, Superconducting, Thinfilm Coatings for RF Accelerator Cavities - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Alameda Applied Sciences Corporation Contact Dr. Mahadevan Krishnan, (510) 483-4156

SQUID-based Nondestructive Testing Equipment of Dished Niobium Sheets for SRF Cavities - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Amac International, Inc. Contact Ian Phipps, (757) 249-3595

Improved Nb For Superconducting RF Cavities - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Shear Form, Inc. Contact Dr. Karl Ted Hartwig, (979) 693-4102

High Z Droplets -- A Novel Source of Heavy Ions for Nuclear Physics - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Tech-X Corporation Contact Dr. John R. Cary, (303) 448-0728

Germanium-76 Isotope Separation by Cryogenic Distillation - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Medical Isotopes, Inc. Contact Eric Stohler, (603) 635-1722

Three-Dimensional High-Resolution Gamma Ray Detector for RIA - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Nova R&D, Inc. Contact Dr. Tumay O. Tumer, (951) 781-7332

Segmentation of the Outer Contact on P-Type Coaxial Germanium Detectors - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; PHDS Contact Dr. Paula Pehl, (510) 845-3144

Fast, Dense, Low Cost Scintillator for Nuclear Physics - DOE Contact Manouchehr Farkhondeh, (301) 903-4398; Radiation Monitoring Devices, Inc. Contact Dr. Gerald Entine, (617) 668-6800

Combinatorial Approach for the Discovery of New Scintillating Materials - DOE Contact Frances Keel, (202) 586-8329; Ajjer, LLC Contact Dr. Anoop Agrawal, (520) 321-7680

FY 2005 PHASE II (FIRST YEAR)

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

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 2005 PHASE II (SECOND YEAR)

Situational Awareness Monitor for Nuclear Events - DOE Contact Frances Keel, (202) 586-2187; ADA Technologies, Inc. Contact 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 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 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 Steven Winter, (203) 857-0200

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

Magnetized Electron Transport in the Proposed Electron Cooling Section of the Relativistic Heavy Ion Collider - DOE Contact Manouchehr Farkhondeh, (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 Manouchehr Farkhondeh, (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 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 Linda L. Even, (757) 930-1463

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

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

NLC Marx Bank Modulator - DOE Contact L. K. Len, (301) 903-3233; Diversified Technologies, Inc. Contact 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 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

MATERIALS STRUCTURE AND COMPOSITION

FY 2005 PHASE I

Nano Graphene Plate-Reinforced Polymer Composites - DOE Contact Charlie Russomanno, (202) 586-7543; Nanotek Instruments, Inc. Contact Dr. Wen C. Huang, (701) 277-1772

Advanced Tungsten Structures for Plasma-Facing Components in Magnetic Confinement Fusion Energy Reactors - DOE Contact Gene Nardella, (301) 903-4956; Ultramet Contact Craig N. Ward, (818) 899-0236

FY 2005 PHASE II (FIRST YEAR)

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

SMALL BUSINESS TECHNOLOGY TRANSFER RESEARCH PROGRAM

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

FY 2005 PHASE I

An Advanced Power Converter System Using High Temperature, High Power Density SiC Devices – DOE Contact Imre Gyuk, (202) 586-1482; Aegis Technology Contact Robert Liu, (714) 265-1238

Economical High Performance Thermoplastic Composite Bipolar Plates – DOE Contact Donna Ho, (202) 586-8000; NanoSonic, Inc. Contact Dr. Richard O. Clays, (540) 953-1785

FY 2005 PHASE II (FIRST YEAR)

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

FY 2005 PHASE II (SECOND YEAR)

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

FY 2005 PHASE I

Property Measurement and Improved Strength of Duplex SiC/Sic Ceramic Composites for Fast Reactor Fuel Cladding – DOE Contact Sue Lesica, (301) 903-8755; Gamma Engineering Corporation Contact Herbert Feinroth, (301) 840-8415

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

FY 2005 PHASE I

Ultra-high Productivity Metal Membranes for Hydrogen Production Applications – DOE Contact Charles Russomanno, (202) 586-7543; Hy9 Corporation Contact Dr. Ann Oppenheimer, (617) 576-6849

Development of Low Cost Conducting Polymer for Electrostatic Precipitators – DOE Contact Charles Russomanno, (202) 586-7543; Applied Sciences, Inc. Contact Max L. Lake, (937) 755-2020

High-Energy-Density Nanocomposite Nd-Fe-B/Fe Magnets for Advanced Generator/Motor Applications - DOE Contact James Ahlgrimm, (202) 586-9806; FutureTek USA Corporation Contact Youngson He, (937) 393-8862

FY 2005 PHASE II (SECOND YEAR)

Nanostructured Polymeric Heterogeneous Catalyst for Industrial Applications - DOE Contact Charles Russomanno, (202) 586-7543; TDA Research, Inc. Contact 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

INSTRUMENTATION AND FACILITIES

FY 2005 PHASE I

Reverse Emittance Exchange for Muon Colliders - DOE Contact Lek K. Len, (301) 903-3233; Muons, Inc. Contact Dr. Rolland O. Johnson, (757) 870-6943

FY 2005 PHASE II (FIRST YEAR)

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

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

174. VANADIUM ALLOY AND INSULATING COATING RESEARCH
$900,000
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

175. THEORY AND MODELING
$1,900,000
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 micro structural 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 c) plastic instabilities and fracture processes in materials irradiated under projected fusion conditions, and d) effects of the many materials, irradiation, and mechanical loading parameters on flow and fracture processes to establish understanding of controlling mechanisms. Techniques include atomistic computer simulation, atomic cluster modeling, Monte Carlo analysis, 3-D dislocation dynamics and flow and fracture models. Research includes materials and conditions relevant to inertial fusion systems as well as magnetic systems.

Keywords: Modeling, Simulation, Irradiation Effects

176. FERRITIC/MARTENSITIC STEEL RESEARCH
$2,200,000
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

177. SiC/SiC COMPOSITES RESEARCH
$1,600,000
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 on the evaluation of improved fibers and alternative interface layer materials. Critical issues include irradiation-induced reduction in thermal conductivity, leak tightness, joining and helium effects. Work on this material class involves irradiation in fission reactors, including HFIR and other test reactors, as partial simulation of the fusion environment. A modeling activity complements the experimental measurements.

Keywords: Silicon Carbide, Composites, Irradiation Effects

178. PLASMA FACING MATERIALS RESEARCH
$2,000,000
DOE Contact: G. Nardella, 301-903-4956
SNLA Contact: R. Nygren, 505-845-3135

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

179. PHYSICAL, CHEMICAL AND STRUCTURAL EVOLUTION OF ZEOLITE-CONTAINING WASTE FORMS PRODUCED FROM METAKAOLINITE AND CALCINED HLW
$205,000
DOE Contact: Roland F. Hirsch, (301) 903-9009
Pennsylvania State University Contact:
Michael Grutzeck, (814) 863-2779
Savannah River National Laboratory 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

180. INVESTIGATING ULTRASONIC DIFFRACTION GRATING SPECTROSCOPY AND REFLECTION TECHNIQUES FOR CHARACTERIZING SLURRY PROPERTIES
$268,000
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

181. CHEMISTRY OF ACTINIDES IN MOLTEN GLASSES AND ITS CORRELATION TO STRUCTURAL PERFORMANCE OF SOLID GLASSES: FILLING THE KNOWLEDGE GAP
$136,000
DOE Contact: Roland F. Hirsch, (301) 903-9009
Oak Ridge National Laboratory Contact: Sheng Dai, (865) 576-7307
Savannah River National Laboratory 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

182. STABILITY OF HIGH LEVEL RADIOACTIVE WASTE FORMS
$330,000
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

183. UNDERGROUND CORROSION AFTER 32 YEARS:A STUDY OF FATE AND TRANSPORT
$260,000
DOE Contact: Roland F. Hirsch, (301) 903-9009
Idaho National 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 2005
OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY GRAND TOTAL	$11,272,340
OFFICE OF SPACE AND DEFENSE POWER SYSTEMS	$6,827,340
SPACE AND NATIONAL SECURITY PROGRAMS	$6,827,340
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$3,813,000
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	3,228,000
Carbon-bonded Carbon Fiber Insulation Production, Maintenance, Manufacturing Process Development, and Product Characterization	585,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING	$3,014,340
Alloy Development Characterization, Mechanical Property Testing, and Insulation	1,577,340
Heat Source Fabrication Development and Materials Testing	1,437,000
OFFICE OF ADVANCED NUCLEAR RESEARCH	$4,445,000
ADVANCED FUEL CYCLE INITIATIVE	$1,815,000
Radiation Damage Modeling in AFCI Materials	310,000
Lead Alloy Technology	1,029,000
Structural Materials Testing	476,000
NUCLEAR HYDROGEN INITIATIVE	$2,630,000
Development of Advanced High-Temperature Heat Exchangers	2,630,000

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

184. 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
$3,228,000
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 2005, 307 flight quality iridium alloy blanks were produced and transferred to the CVS Production Task. Forty-eight kilograms of iridium powder was qualified for iridium blank production. One hundred twenty five prime quality iridium alloy CVSs and eleven “engineering use” CVSs were completed and shipped in FY 2005. The Annual Iridium Inventory Report was issued.

Keywords: Iridium Processing, Melting, Extrusion, Clad Vent Sets

185. CARBON-BONDED CARBON FIBER INSULATION PRODUCTION, MAINTENANCE, MANUFACTURING PROCESS DEVELOPMENT, AND PRODUCT CHARACTERIZATION
$585,000
DOE Contact: John Dowicki, (301) 903-7729
ORNL Contacts: Jim King, (865) 574-4807, Glenn Romanoski, (865) 574-4838

The Carbon-Bonded Carbon Fiber (CBCF) production facilities have been operated in a production maintenance mode since the Cassini campaign to produce flight quality insulators sets. Dedicated facilities and trained personnel for the CBCF production remain in the Carbon Materials Technology Laboratory at ORNL. Twenty-four prime quality CBCF insulator sleeves and forty-eight discs were produced during FY 2005. These sleeves meet all property requirements. Technical support was provided to the GPHS Aeroshell Materials Working Group for near-term procurement and determining a future path for obtaining Fine-Weaved Pierced Fabric material.

Keywords: Insulation/Thermal, Carbon-Bonded Carbon Fiber, Carbon Fibers

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERISTICS OR TESTING

186. ALLOY DEVELOPMENT CHARACTERIZATION, MECHANICAL PROPERTY TESTING, AND INSULATION
$1,577,340
DOE Contact: John Dowicki, (301) 903-7729
ORNL Contacts: Jim King, (865) 574-4807, Easo George, (865) 574-5085, John Shingledecker, (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 2005. Tensile impact testing was performed on DOP-26 iridium alloy to study the effect of grain size on ductility in the range of 500-900˚C. Testing continued to determine the influence of oxygen on the tensile properties of Ta-10W alloy over a range of temperatures. The effect of aging on the embrittlement of Haynes 25 alloy was also studied.

Capsule pressure-burst and coupon creep rupture testing continued 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 completed.

Testing continued 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

187. HEAT SOURCE FABRICATION DEVELOPMENT AND MATERIALS TESTING
$1,437,000
DOE Contact: John Dowicki, (301) 903-7729
ORNL Contacts: Jim King, (865) 574-4807 and 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 the capsule and all other components for the heat source. ORNL is also conducting a materials testing program to produce a mechanical property data base to support the analyses of materials performance and design requirements.

Heat source capsules and other components were produced to support welding development and planned testing activities. Refurbishment of ultra-high vacuum creep machines was completed and capsule pressure burst machines were assembled. Creep and tensile testing of Ta-10W and other material specimens was performed.

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.

188. RADIATION DAMAGE MODELING IN AFCI MATERIALS
$310,000
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

189. LEAD ALLOY TECHNOLOGY
$1,029,000
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

190. STRUCTURAL MATERIALS TESTING
$476,000
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.

191. DEVELOPMENT OF ADVANCED HIGH-TEMPERATURE HEAT EXCHANGERS
$2,630,000
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 degrees 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 2005
NATIONAL NUCLEAR SECURITY ADMINISTRATION GRAND TOTAL	$118,126,000
OFFICE OF NAVAL REACTORS	$66,600,000[1]
OFFICE OF DEFENSE PROGRAMS	$51,526,000
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM	$51,526,000
SANDIA NATIONAL LABORATORIES	$34,066,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$7,946,000
Assembly and Actuation of Nanomaterials Using Active Biomolecules	500,000
Decomposition of Contaminants Using Photochemically Active Nanoparticles	460,000
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	315,000
Nanolithography Directed Materials Growth and Self-Assembly	470,000
Novel Gel-Based Technology for Sensors and Weapons	100,000
Developing the Foundation for Polyoxo-Niobate Chemistry: Highly Tunable and Exploitable Materials	250,000
Physics & Chemistry of Ceramics	695,000
Field-Structured Anistropic Composites and Complex and Cooperative Phenomena in Disordered Ferroelectrics and Dielectrics	462,000
Artificially Structured Biocompatible Semiconductors	481,000
Atomic Processes and Defects in Wide-Bandgap Semiconductors	362,000
Advanced Growth Techniques and the Science of Epitaxy	295,000
Active Assembly of Dynamic and Adaptable Materials	900,000
Synthesis and Processing of Nanoclusters for Energy Applications	450,000
Dipolar Nanocomposites	170,000
Cooperative Phenomena in Molecular Nanostructures	635,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$18,936,000
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	445,000
Coupled Nanomechanical Oscillator Arrays for the Study of Internal Dissipation in Nano-Scale Structures and Collective Behavior in Large Systems	310,000
Atomic Level Science of Adhesion and Interfacial Wetting	593,000
Mechanical Properties of Nanostructured Materials	227,000
Localized Corrosion Initiation at Nanoengineered Defects in Passive Films	578,000

[1]This excludes $67.5 million for the cost of irradiation testing in the Advanced Test Reactor (ATR).

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2005
OFFICE OF DEFENSE PROGRAMS (continued)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (continued)	
SANDIA NATIONAL LABORATORIES (continued)	
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING (continued)	
The Science of Electronic and Optical Interactions Between Coupled Nanostructures	950,000
Materials Aging and Analytical Technique Development	4,500,000
Scientifically Tailored Materials and Materials Processing	4,500,000
MATERIALS STRUCTURE AND COMPOSITION	$3,844,000
Modeling of Friction-Induced Deformation and Microstructure	500,000
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	161,000
Long Range Particle Interactions and Collective Phenomena in Plasma Crystals	347,000
Atomistic Basis for Surface Nanostructure Formation	350,000
DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING	$3,340,000
Advanced Packaging/Joining Technology for Micro	375,000
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	300,000
Diatoms as Molecular Architects	350,000
Novel Mechanisms of Nanomechanical and Transmembrane Actuation	350,000
Carbon Nanotube Sorting via DNA-Directed Self-Assembly	300,000
Next-Generation Contact Materials for High-Reliability Microsystems Devices	380,000
Controlled Fabrication of Nanowire Sensors	435,000
Fundamental Enabling Issues in Nanotechnology: Stress at the Atomic Level	300,000
Effective Dispersion of Nanoparticles by Polymers	200,000
LAWRENCE LIVERMORE NATIONAL LABORATORY	$8,100,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$8,100,000
Engineered Nanostructure Laminates	6,200,000
AFM Investigations of Biomineralization	200,000
Beryllium Ablator Coatings for NIF Targets	1,400,000
Plasma Polymer Coating Technology for ICF Targets	300,000

NATIONAL NUCLEAR SECURITY ADMINISTRATION

	FY 2005
OFFICE OF DEFENSE PROGRAMS (continued)	
THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM (continued)	
LOS ALAMOS NATIONAL LABORATORY	$9,360,000
CAMPAIGN 8 AND THE JOINT MUNITIONS PROGRAM (DOD/DOE)	$9,360,000
Enhanced Surveillance of High Explosives	3,070,000
MIC Project	389,000
High Explosive Crystal Growth and Characterization	225,000
Damage in Mock Explosive Materials	75,000
Shock Initiation Experiments on the TATB Based Explosive PBX 9502: Comparison of Baseline and Aged Materials	375,000
Dynamic Behavior of Polymers and Foams	625,000
Explosives Chemistry and Properties	501,000
Microstructural and Kinetic Effects on the Behavior of Energetic Materials	950,000
Proton Radiography of a Thermal Explosion in PBX 9501	600,000
Thermal Response of PBX 9501	300,000
JMP: Polymer Behavior Under Dynamic Loading	1,000,000[1]
Thermal and Loading Dynamics of Energetic Materials	1,250,000

[1]The joint DOE and DoD contribution

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 $134.1 million in FY2005. Approximately $67.5 million represents the cost for irradiation testing in the Advanced Test Reactor. The Naval Reactors contact is Weston J. Pollock, (202) 781-6141.

OFFICE OF DEFENSE PROGRAMS

THE WEAPONS RESEARCH, DEVELOPMENT AND TEST PROGRAM

SANDIA NATIONAL LABORATORIES

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

192. 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 nanocrystal quantum dot (nQD) arrays through modulation of inter-particle spacing. Here, the spacing between different sized nQDs 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 processes 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 materials in complex systems.

Keywords: Biomolecules, Nanowires, Nanoparticles, Functional Assemblies

193. DECOMPOSITION OF CONTAMINANTS USING PHOTOCHEMICALLY ACTIVE NANOPARTICLES
$460,000
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 (TiO2, ZnO, Fe2O3, WO3) 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. The ultimate outcome of this work will be the development of a new class of highly active materials for wide ranging decontamination applications.

Keywords: Nanoparticles, Photo-Active, Materials Synthesis, Decontamination

194. 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. We believe that 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. We have successfully synthesized a wide range of cleavable surfactants over the past eighteen months that will function as removable templates. We have determined that all of the surfactants synthesized behave as traditional amphiphiles and have characterized their static and dynamic properties. Observations indicate that the surfactants degrade upon initiation of the appropriate trigger and lose their surface-active properties. We have utilized these surfactants in proof-of-concept experiments that involve emulsion polymerizations using these labile assemblies as scaffolding agents.

Keywords: Surfactuants, Mesoporous, Materials Synthesis, Diels-Alder

195. 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

Solid progress has been made in the first two years of this LDRD work. The enhanced hydrogen sorption kinetics present in Ti-doped sodium alumninum hydride have been the focus of investigation. Competing models developed for the rate limiting step of hydrogen sorption include surface enhancement of hydrogen dissociation due to the presence and dispersion of titanium on aluminum surfaces, and possible bulk effects such as lowering of nucleation barriers and interfacial free energies, allowing phase transitions to occur more rapidly between the decomposition products of $NaAlH_4$.

Previous studies have determined that substitution of titanium on lattice sites of Na and Al in bulk NaAlH4 is unlikely due to total energy considerations and x-ray diffraction data from single crystals of NaAlH4 exposed to titanium during growth. This does not rule out the possibility of defect-induced stability for Ti substitution. Previous first-principles work has also shown that defect structures involving Ti can be stable, such as Ti on an Al site, with a hydrogen vacancy.

A combination of experiments is proposed for the last year to determine which, and possibly if both, mechanisms are responsible for the enhanced kinetics. Hydrogen sorption experiments using well-known catalysts as hydrogen dissociators will be used to determine the dissociation effeciency of Ti-dopants, yielding information on surface kinetics models. In addition, Raman spectroscopy of both single crystals and doped and undoped powders of NaAlH4 will directly probe the Al-H bond strength and aluminum coordination in these materials. This will give direct information on defect structures that may be present in doped alanates. This work will also be useful for other compounds where Al-H coordination is needed.

We propose to determine which of the kinetics enhancement models offers the greatest increase in sorption kinetics, and if these enhancements are possible to carry over to related hydrides.

Keywords: Catalysis, Thermodynamics, Metal-Hydrides, Hydrogen Storage

196. 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:

- To develop new methods to assemble ordered conducting materials on multiple length scales. Both self-assembly and directed nucleation and growth approaches will be explored to produce oriented and aligned polymer nanostructures and microstructures

- To establish fundamental structure-property relationships of nanostructured conjugated polymers. We propose to investigate films in which conjugated polymers and polymer-nanocrystal composites are confined to ordered structures with 1-, 2-, or 3-dimensional connectivity and separated by either insulating or semiconducting walls. Such composites are ideal model systems in which to test and understand the role of nanostructuring in determining charge and energy transport properties.

- To integrate the new materials/structures with microelectronic/microfluidic devices. This strategy holds the promise for inexpensive electronic/optical devices. Micro-arrays of such materials will also be developed for quantitative and high sensitivity detection of chemical and biological agents.

The proposed research will not only contribute to our new strategy thrust in complex functional materials, it will also have a positive impact on DOE's missions in energy and national security.

Keywords: Bioactive Materials, Electro-Optics, Microelectronics, Microfluides, Functional Materials

197. 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 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

198. DEVELOPMENT OF HIGH ENERGY DENSITY DIELECTRIC MATERIALS FOR INTEGRATED MICROSYSTEMS
$315,000
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 dielectric constant (K) = 1100 dielectrics:

- 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.

- 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, CaCu3Ti4O12, Ca:K(Ta,Nb)O3, and (Pb,La)TiO3, dielectric constants of 12,000 to 280,000 that are stable over more than a 300˚C 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

199. NANOLITHOGRAPHY DIRECTED MATERIALS GROWTH AND SELF-ASSEMBLY
$470,000
DOE Contact: Mike Long, (202)586-4595
SNL Contact: Julia W. P. Hsu, (505)284-1173

The goal of this LDRD is to integrate nanotechnology and inorganic materials growth/assembly for potential applications in bio/chemical sensing, optoelectronics, catalysis, and novel microsystems. To include these inorganic materials in micro-devices and microsystems, they will need to be positioned on the substrates in a controlled and pre-determined fashion. Our approach to this goal is from “bottom-up” rather than “top-down,” in which conventional optical and electron-beam lithography function. We adapt soft nanolithography techniques to selectively modify the growth surfaces chemically with organic molecules to enhance or inhibit crystal nucleation, which in turn determines the final spatial organization of inorganic crystals. Such an approach is purely additive, i.e. depositing materials only where they are desired, and avoids contaminating the pristine nature of substrate surfaces. These chemically patterned surfaces are then used as templates for nano-crystal growth through bio-inspired approaches in aqueous solutions. In addition to spatial selectivity, the crystal orientation can be controlled through the different chemical or physical structure of the patterned surfaces. Crystal morphology and hierarchical structures can be tuned through solution chemistry and growth conditions. We have already successfully demonstrated the approach described above in selective growth of ZnO nano-rods on Ag surfaces. In principle, this approach is applicable to a wide variety of inorganic crystals and substrates, depending on the desired applications. With the progress made in FY04 and the proposed future work outlined here, 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

200. 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 of this LDRD is to develop a fundamental understanding the volume phase transition in non-aqueous polymer gels. The research will have two applications. First, this work will provide a foundation necessary to launch Sandia into sensor development for chemical and biological agents, a likely arena relevant to homeland defense initiatives. Second, the research is essential for developing materials solutions for new gel based capacitors proposed in 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 and kinetics of the phase transition and the impact of the polymer structure on the transition so that the above challenges can be met and intelligent materials designed. For weapons, 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 capacitors in the firing sets. A critical aging mechanism for these capacitors is solvent partitioning in the margin-fill gel. A scientific understanding of this partitioning is critical for accurate prediction of capacitor lifetime and design of gel materials with improved capacitor performance.

Keywords: Polymer, Polymer Gels, Capacitors, Analyte Absorption, Phase Transition

201. DEVELOPING THE FOUNDATION FOR POLYOXO-NIOBATE CHEMISTRY: HIGHLY TUNABLE AND EXPLOITABLE MATERIALS
$250,000
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. These different properties of the polyoxoniobates present the opportunity for new applications such as nuclear waste processing and improved performance for metal and virus binding.

The purpose of research is to 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 nuclear magnetic resonance (NMR) 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. 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 inito structure determination from powder diffraction as a core capability.

Keywords: Polyoxometalate, Polyoxoniobates, NMR

202. PHYSICS & CHEMISTRY OF CERAMICS
$695,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: C. Jeffery Brinker, (505) 272-7627

The goal of the project 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 relationships.

Keywords: Ceramics, Molecular Precursors, Self-Assembly

203. FIELD-STRUCTURED ANISTROPIC COMPOSITES AND COMPLEX AND COOPERATIVE PHENOMENA IN DISORDERED FERROELECTRICS AND DIELECTRICS
$462,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: J. E. Martin, (505) 844-9125 and George Samara, (505) 844-6653

<u>Task 1: Field-Structured Anisotropic Composites</u>

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 complex dielectrics, ferroelectrics and relaxors and of the mechanisms for ferroelectric-to-relaxor crossover in compositionally-disordered ferroelectrics. Some emphasis is (i) on dipolar impurities in quantum paraelectrics and the onset of dipolar correlations, and (ii) the origin of giant dielectric constants. 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 ® 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 to provide revealing insights into the physics.

Keywords: Cooperative Phenomena, Ferroelectrics, Field-Structured Composites, Ferroelectric-to-Relaxor

204. ARTIFICIALLY STRUCTURED BIOCOMPATIBLE SEMICONDUCTORS
$481,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: P. L. Gourley, (505) 844-5806

This project investigates biocompatible semiconductor micro/nanocavities for optical sensing of biomolecules and cells. The scope 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.

Keywords: Biocompatible Semiconductor, Micro/Nanocavities, Microfluids, Optical Transduction

205. ATOMIC PROCESSES AND DEFECTS IN WIDE-BANDGAP SEMICONDUCTORS
$362,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: S. M. Myers, (505) 844-6076

Our objective is fundamental understanding of the atomic processes and point defects that limit the properties of wide-bandgap compound semiconductors. We use a variety of electrical, spectroscopic, and ion-beam analyses to characterize solute and defect states and observe their behavior under stimuli such as heating, voltage bias, and ion and electron irradiation. Results are interpreted through quantitative modeling based on *ab-initio* theory to achieve a unified, predictive description of behavior. The principal current focus is on GaN and its alloys, with particular attention to issues affecting p-type doping. Properties under study include the configurations, state energies, diffusion, and bound complexes of H, other impurities, dopants, and interstitial and vacancy defects.

Keywords: Point Defects, Wide-Bandgap Compound Semiconductors, Ab-Initio theory, GaN, ZnO

206. ADVANCED GROWTH TECHNIQUES AND THE SCIENCE OF EPITAXY
$295,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: 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

207. ACTIVE ASSEMBLY OF DYNAMIC AND ADAPTABLE MATERIALS
$900,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: B. C. Bunker, (505) 284-6892

The objective of this project is to learn how to exploit proteins that consume energy to mediate polymerization/depolymerization and active transport processes to assemble or reconfigure nanocomposite materials. Such active assembly processes should facilitate the fabrication of non-equilibrium structures that are difficult or impossible to create using standard self-assembly processes. The project currently is focused on learning how to stabilize and control both microtubules and the motor protein kinesin to direct the active transport and assembly of nanomaterials in extra-cellular environments.

Keywords: Microtubules, Motor Proteins, Nanoparticles, Active Transport, Self-Organized

208. SYNTHESIS AND PROCESSING OF NANOCLUSTERS FOR ENERGY APPLICATIONS
$450,000
DOE Contact: Richard Kelley, (301) 903-6051
SNL Contact: 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 and photocatalysis. We use feedback from studies of the cluster physical properties to refine our synthetic protocols.

Keywords: Semiconductor Nanoclusters, Size-Dependent Properties

209. DIPOLAR NANOCOMPOSITES
$170,000
DOE Contact: Richard Kelley, (301) 903-6051
SNL Contact: J. E. Martin, (505) 844-9125

The goal of this project is to develop and investigate a class of complex materials we call dipolar nanocomposites, that consist of superparamagnetic (or superparaelectric) nanoclusters organized into complex structures 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

210. COOPERATIVE PHENOMENA IN MOLECULAR NANOSTRUCTURES
$635,000
DOE Contact: Richard Kelley, (301) 903-6051
SNL Contact: D. Y. Sasaki, (925) 294-2922

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

211. 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 (mechanical and fatigue strength, interfacial friction and stiction, electrical resistance). Eventually, device function is clearly threatened and, as such, these aging processes have the potential for high (negative) consequence.

Currently, no reliable information exists on the critical species (and concentration levels) that will be present within the sealed packages or on component surfaces. The analytical techniques to properly perform the needed characterization activities on these environments do not exist. The goal is to develop a set of tools that are analytical strategies and methods to measure the spatially resolved chemical inventory within Sandia fabricated and packaged microsystems. These tools can be broadly subdivided into surface and internal gas atmosphere characterization, with the aid of multivariate data processing. Both require the design and fabrication of a suitable MEMS test platform capable of being opened easily and cleanly. Surface characterization involves tagging known contaminants in order to enhance surface analyses, and multivariate analyses of merged data from different surface analysis techniques. 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 to characterize the package vapor phase. We will develop and apply new multivariate statistical techniques to spatially resolved ion, x-ray and optical spectroscopies to identify and quantify the spatial distribution of critical surface species (e.g., lubricants, anti-stiction reagents) and contaminants. Tools developed in this work will enable the acquisition and processing of surface/gas data to support design of integrated state-of-health sensors, identify important degradation/dormancy mechanisms, establish packaging specifications to assure adequate weapons reliability, and establish future surveillance methods.

Keywords: Materials Aging, MEMS, Microelectro-mechanical, Packaging, Surface Analysis, Chemical Analysis

212. 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 need for improved understanding of dynamic solidification behavior under high pressures. We propose to study the solidification transition in tin under isentropic compression.

We have developed a new empirical potential and begun large-scale molecular-dynamics simulations of solidification in tin using this potential. Proposed continuing work will focus on using these simulations to investigate the kinetics of solidification in both the nucleation and growth phases. We continued preliminary analyses of previous experiments on ramp-wave compression of liquid tin, and continue to work on improving the experiment design. Proposed continuing work will investigate the equation-of-state (EOS) for tin and attempt to develop a continuum-level model for kinetics of the solidification process that incorporates results from molecular-dynamics simulations.

This research will develop future capability and expertise in a novel area of materials dynamics characterization that is of high interest to stockpile stewardship, beyond the scope of existing programmatic work (the latter focuses on obtaining experimental data rather than understanding those data). The results will also improve the fundamental understanding of solidification processes, aiding both the prediction of material behavior under dynamic loading and the modeling of more traditional processes such as welding and soldering.

Keywords: Phase Transition, Freezing, Tin, Dynamic Compression, Molecular Dynamics

213. ELECTROCHEMICALLY SWITCHABLE MATERIALS FOR (BIO)MICROFLUIDICS
$200,000
DOE Contact: Mike Long, (202)586-4595
SNL Contact: Kevin R. Zavadil, (505)845-8442

Homeland security needs require the development of a new generation of microfluidic devices that can concentrate, separate and sense a variety of viral, bacterial and toxic agents. The key enabler are functional materials capable of being programmed to perform a wide variety of operations on complex biological samples and that are compatible with nanoscale architectures. 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 beta-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 microelectromechanical (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, 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

214. 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

We propose a multi-part project to select and obtain a weaponized /non-weaponized simulant of anthrax and analyze the same specific region of simulant material with multiple analytical techniques. In parallel, we will characterize the range of analytical techniques with simple test specimens and with MSA tools that will be developed to augment our Automated eXpert Spectral Image Analysis (AXSIA) software. Additionally, and most importantly new algorithms will be developed and tested for multiple correlated analyses. The outcome will be a comprehensive and correlated analytical protocol as well as tools for performing analysis of bio- or other agents.

The analytical techniques included can be grouped into three categories: bulk methods (Gas/Liquid Chromatography with Mass Spectrometry and Laser Induced Breakdown Spectroscopy); surface methods (X-ray Photoelectron Spectroscopy, Auger Electron Spectroscopy, and Time of Flight Secondary Mass Spectrometry); and microanalytical methods (electron, x-ray and particle excited x-ray microanalysis, IR, Raman and Visible Spectroscopy).

The analytical data analysis method, which is based upon multivariate statistical analysis, will build upon the previously developed AXSIA software to read new data types, perform calculations optimized for new analytical techniques, and perform correlated analyses.

Keywords: Multivariate, Spectral Image Analysis

215. 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 under atmospheric conditions relevant to the anticipated service conditions. 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

216. 3D OPTICAL SECTIONING WITH A NEW HYPERSPECTRAL DECONVOLUTION FLUORESCENCE IMAGING SYSTEM
$445,000
DOE Contact: Mike Long, (202)586-4595
SNL Contact: David M. Haaland, (505)844-5292

This project includes designing, building, and applying a novel hyperspectral deconvolution fluorescence microscope for 3D diffraction-limited optical sectioning of cells and subcellular organelles, 3D monitoring of microfluidic processes, and investigation of molecular motors. We are developing data analysis methods to deconvolve the hyperspectral image data and to rapidly extract 3D concentration distribution maps of all emitting species. The imaging system has 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 can improve both spectral and spatial deconvolution processes. The system can make rapid survey scans of large areas followed by detailed 3D 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) 3D composition mapping analysis of multicomponent microfluidic processes such as mixing, dispersion, and chemical syntheses of materials, 2) quantitative analysis and co-localization of molecular motors in 3 dimensions, and 3) examining the binding of functionalized lipid vesicles to specific cells and the release and/or internalization of the vesicle contents. The project is on schedule and has met all milestones. This challenging project, when successful, will make Sandia a major player in advanced spectral imaging techniques for materials research, sensor technology, and biotechnology.

Keywords: Hyperspectral, Fluorescence, Microfluidic, Confocal Imaging, Multivariate

217. COUPLED NANOMECHANICAL OSCILLATOR ARRAYS FOR THE STUDY OF INTERNAL DISSIPATION IN NANO-SCALE STRUCTURES AND COLLECTIVE BEHAVIOR IN LARGE SYSTEMS
$310,000
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

218. ATOMIC LEVEL SCIENCE OF ADHESION AND INTERFACIAL WETTING
$593,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: 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 develop predictive models for adhesive bond strength, interfacial stability and flow kinetics; and tailor material surfaces for optimized adhesion, wetting or lubrication.

Keywords: Adhesion, Wetting, Interface Formation, Interfacial Stability

219. MECHANICAL PROPERTIES OF NANOSTRUCTURED MATERIALS
$227,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: D. M. Follstaedt, (505) 844-2102

Our goal is to understand the basic deformation properties of nanostructured materials and the evolution of stress in them. We identify the fundamental strengthening mechanisms and quantify the mechanical properties of metals with ~1-100 nanometer internal structures (grains, voids, second phases), and determine the fundamental causes of stress during the growth of thin films. We use special methods to synthesize materials designed to elucidate these mechanisms (electrodeposition, lithography, pulsed-laser deposition (PLD) and ion implantation), develop advanced methods for characterization (nanoindentation + finite-element modeling, MEMS-based devices), and use in situ methods to obtain the most direct information (TEM during straining, specimen curvature during growth). These approaches provide fundamental new insights into nanomaterials.

Keywords: Deformation, Stress Evolution, Laser Deposition, *In Situ* Examinations

220. LOCALIZED CORROSION INITIATION AT NANOENGINEERED DEFECTS IN PASSIVE FILMS
$578,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contacts: N. A. Missert, (505) 844-2234 and
J. Charles Barbour, (505) 844-5517

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

221. THE SCIENCE OF ELECTRONIC AND OPTICAL INTERACTIONS BETWEEN COUPLED NANOSTRUCTURES
$950,000
DOE Contact: Richard Kelley, (301) 903-6051
SNL Contact: M. P. Lilly, (505) 844-4395

This research project investigates the interactions between coupled nanoelectronic and nanophotonic structures. We are addressing the following general questions: What novel types of behavior, including collective behavior, ensue from different types of strong interactions, e.g., photon and electron tunneling, Coulomb, and exchange? How sensitive is the behavior to geometry, interaction strength, and temperature? How well can it be controlled and manipulated? What new methods of materials growth, patterning, and synthesis will enable creation of large, strongly interacting arrays of nanostructures? How can interfacing with the macro-world best be accomplished?

Keywords: Fractional Quantum Hall Effect, Nanoelectronic, Nanophotonic, Coulomb Exchange, Hybrid Interactions

222. 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 Anlaysis, Information Extraction

223. 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

MATERIALS STRUCTURE AND COMPOSITION

224. MODELING OF FRICTION-INDUCED DEFORMATION AND MICROSTRUCTURE
$500,000
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 Transmission Electron Microscopy (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

225. 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. The resulting insight into solute effects will enable improved materials design for LIGA alloys and will greatly extend the realism and utility of Sandia's material process modeling capabilities.

Keywords: LIGA, Recrystallization, Grain Growth, Solute Segregation

226. 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

227. THEORY OF MICROSTRUCTURES & DEFORMATION
$161,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: E. A. Holm, (505) 844-7669

The goal of this project is to combine experiment, modeling, and simulation to construct, analyze, and utilize three-dimensional (3D) polycrystalline microstructures. Novel algorithms construct 3D polycrystals to match an arbitrary number of microstructural parameters. These 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.

Keywords: Microstructures, Microstructural Network Parameters, Grain and Subgrain, Deformation

228. LONG RANGE PARTICLE INTERACTIONS AND COLLECTIVE PHENOMENA IN PLASMA CRYSTALS
$347,000
DOE Contact: Yok Chen, (301) 903-4174
SNL Contact: G. 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 methods to describe the many-body interactions that govern these crystals, including experimental diagnostics to characterize particle temperatures and the interparticle potentials as well as models to describe these 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

229. ATOMISTIC BASIS FOR SURFACE NANOSTRUCTURE FORMATION
$350,000
DOE Contact: Richard Kelley, (301) 903-6051
SNL Contact: G. L. Kellogg, (505) 844-2079

The goal of this project is to establish the scientific principles governing the formation and stability of nanostructures on surfaces. Our current efforts focus on understanding how atomic-scale, kinetic processes control collective phenomena on surfaces such two-dimensional pattern formation, surface smoothing, surface alloying, and 3-d cluster diffusion. Our approach is to 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 move and interact on surfaces. From these studies we obtain new insights into the complex physics that takes place during the formation and evolution of surface structures at length scales relevant to the emerging nanotechnologies.

Keywords: Collective Surface Phenomena, Surface Self-Assembly, Thermal Smoothing, Surface Structure

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

230. ADVANCED PACKAGING/JOINING TECHNOLOGY FOR MICRO
$375,000
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. Two complementary new technologies have been identified - micron-scale high energy density (HED) fusion welding and focused-ion-beam deposition joining (FIBDJ) - that can jointly address these key microsystem needs. At the micron scale, materials properties which dominate joining response differ appreciably 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. Techniques for producing the fine scale beams are being developed, and these power sources are being characterized spatially and temporally, and in terms of energy transfer. Previous modeling showed 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 are using Molecular Dynamics simulations to provide surface tensions. Surface Evolver (SE) and GOMA simulations are being used to 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 modeling. The models are being 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 in both processes and will be addressed at the latter stages of the project.

Keywords: Advanced Packaging, Microscale Welding, MEMS, Focused Ion Beam

231. 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

232. REVERSIBLE ANTIBODY TRAPPING FOR SELECTIVE SENSOR DEVICES
$200,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Dale L. Huber, (505) 844-9194

For Homeland Security, Sandia needs to develop compact sensors that can selectively detect low concentrations of a wide range of potential biological agents. 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 FTIR, interfacial force microscopy, and neutron scattering (at LANSCE) 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

233. PRECISELY CONTROLLED PICOLITER VESSELS WITH RAPID SAMPLE PREPARATION FOR TRACE BIOTOXIN DETECTION
$300,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: C. R. Bowe Ellis, (925) 294-2158

This project explores the synthesis and characterization of novel microstructures for discrete, controllable sample management in microsystems. Large, synthetic analogues of natural vesicles will enable control over microsamples and microreactions that was previously unattainable. These containers are formed, loaded, moved, and fused to conduct picoliter reactions with exquisite precision. As containers, vesicles are made of an engineerable wall material capable of being selectively permeated yet, when sealed, preventing samples from escaping. As substrates, vesicles are ideal for low reagent volumes and fast surface-dominated reactions required in the preparation of any assay. The applications abound: in biochemistry as a platform for study of molecular dynamics, in chem/bio threat detection as a dilution-free conveyance and preparation motif. Predicated on the paradigm of electrical control, we envision a system boasting vesicle electroformation from lipid primitives, membrane permeation and loading of analytes using electroporation, container fusion with electrical mediation, and vesicle control with electrokinesis. The first steps are embodied in this project. Our objectives are: 1) to synthesize vesicles capable of withstanding electrical and mechanical stressors; 2) to develop an embedded vesicle formation technique; 3) to best our ability to permeate vesicle membranes for sample loading and unloading; 4) to confine and trigger metered reactions within these vesicles; and 5) to demonstrate chip-based movement, filtering, and sensing control over individual vesicles. The culmination of this effort will provide the appropriate biomimetic materials and technology needed to intelligently manage samples for more sensitive and accurate nanodetection.

Keywords: Picoliter, Microfludic, Phospholipid, Electrokinetically, Membrane

234. DIATOMS AS MOLECULAR ARCHITECTS
$350,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Blake Simmons, (925) 294-2288

Current bio-inspired methodologies for the realization of self-assembled nanomaterials are adequate for certain applications, but major breakthroughs are needed for these materials to achieve everyday use. One of the most promising fields of nanotechnology/biotechnology lies in the advent and control of biologically self-assembled materials, especially those involved with silica and other ceramics. Diatoms are eukaryotic algae that are ubiquitous in marine and freshwater environments. They are known to be the dominant form of phytoplankton and are critical to global carbon fixation. Diatoms produce intricate silica structures, known as frustules, during cell division and reproduction that are of two basic types: pennate and centric. Diatoms achieve these structures in exact fashion through genetically inspired design rules coupled with precisely directed biochemistry. We propose to understand and harness the organized silica deposition process that exists in diatoms in order to achieve biologically controlled three-dimensional self-assembly of complex nano- and mesoscale structures.

This project will combine our expertise in materials chemistry, genetics, and computational modeling in order to elucidate the fundamental mechanisms by which these organisms produce these fault tolerant structures. We will then apply this knowledge to produce silica-based structures in a controlled and directed fashion. The first step on this path is to take advantage of available information on the genetic, proteomic, and biochemical basis for diatom silica shape determination and add to that information database through recombinant experimentation and analysis. We will then utilize this knowledge in the laboratory to produce materials that will be fully characterized at the molecular level. We will couple these efforts with a computational evaluation of biologically controlled silica deposition and emergent intercellular phenomena to identify the rudimentary design rules by which these organisms operate. The successful completion of this research will enable advances in the field of self-healing nanomaterials, coatings, photonics, and catalysis.

Keywords: Diatoms, Silica, Biochemistry, Self-assembly

235. NOVEL MECHANISMS OF NANOMECHANICAL AND TRANSMEMBRANE ACTUATION
$350,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Kevin Leung, (505) 844-1588

In nature as in synthetic "smart" materials, local energetic interactions propagate over distances to do mechanical work. Harnessing such energy transduction mechanisms will impact future national security concerns ranging from synthesizing robust, integrated nanosized devices, manipulating nanoparticles on surfaces, and preparing new types of sensors. Synthetic nanotools based on nickel porphyrin triggers are among the simplest energy transduction prototypes. Photoexcitation or chemical binding changes the effective size of the nickel ion, inducing motion in the tightly bound porphyrin ligands and causing nanomechanical motions that can be amplified via specifically tailored structures attached to the porphyrin -- creating nanotweezers. Tightly-bound metal-ligand interactions are also suspected to participate in the actuation (i.e., opening/closing motion) of biological transmembrane ion channels. These channels transmits or blocks electrical signals in response to gating events that can be strongly correlated with channel conformation and selective ion binding. X-ray data exist for the closed K^+ channel from streptomyces lividans (KcsA) configuration, but are "snapshots" and do not fully reveal the complex actuation mechanism. Since certain underlying principles of transmembrane proteins and the simpler porphyrin systems appear similar, and because nickel-porphyrin actuators can potentially be integrated into ion channels to perform gating in response to environmental changes, we propose a joint study. We will use computer modeling assisted synthesis, X-ray crystallography, nuclear magnetic resonance (NMR), Raman, UV-visible absorption, and quantum spectral simulations to obtain a clear understanding of nanomechanical motion in robust, photo- or chemo-triggered porphyrin. We will develop theoretical techniques to treat actuation-induced nanomechanical motion using porphyrins as test cases, and extend them to correlate metal ion (e.g. Na, K, Tl, Rb) size-induced conformational changes in ion channels with large scale channel-opening motion.

Keywords: Nanomechanics, Transduction

236. CARBON NANOTUBE SORTING VIA DNA-DIRECTED SELF-ASSEMBLY
$300,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Amalie Frischknecht, (505) 284-8585

Single-wall carbon nanotubes have shown great promise in novel applications in molecular electronics, biohazard detection, and composite materials. Carbon nanotubes exhibit phenomenal mechanical strength and environment-sensitive electrical properties that range from metallic to semiconducting, depending on tube diameter and helicity. Commercially synthesized nanotubes exhibit a wide dispersion of geometries and conductivities, and tend to aggregate. Hence the key to using these materials is the ability to solubilize and sort carbon nanotubes according to their geometric/electronic properties. Very recent experimental work published in Science has demonstrated that single-stranded DNA will bind to carbon nanotubes, solubilize them in water, and allow sorting of the nanotubes based on their diameter. However, the mechanism for this is not currently understood and most interestingly, depends on the DNA sequence. We propose to investigate DNA/carbon nanotube binding and its dependence on DNA sequence and the solution environment. DNA/nanotube hybrids will be characterized by a variety of techniques including DNA melting experiments, adsorption spectroscopy and atomic force microscopy (AFM). Molecular modeling and simulations will elucidate optimal DNA binding conformations as functions of tube diameter/helicity, DNA sequence, and aqueous ion moiety. Electronic measurements and ab initio and hybrid quantum-mechanics/molecular-mechanics (QM/MM) calculations will explore the effect of DNA on nanotube electronic properties, a crucial step for developing electronic and sensor applications based on carbon nanotubes. Ultimately this work will impact Sandia's mission in science-based materials processing, novel sensors for homeland security, and control of nanosystems

Keywords: Carbon Nanotubes, DNA, Self-assembly

237. NEXT-GENERATION CONTACT MATERIALS FOR HIGH-RELIABILITY MICROSYSTEMS DEVICES
$380,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Paul Vianco, (505) 844-3429

Dynamic electrical contacts are essential micro-electrical mechanical systems (MEMS) devices such as environmental sensing devices (ESDs), switches, and radio frequency (RF) devices. However, microsystems electrical contacts present unique materials challenges because, at the low forces associated with MEMS devices, actual contact occurs at a few surface asperities. Local power densities may exceed 10 kW/cm2, causing temperatures to reach upwards of 1000C. Micro-welding can sticks the contacts together. Also, these elevated temperatures cause excessive oxidation and/or the decomposition of contaminant films, all potentially increasing contact resistance. This study examines the effects of contact force, electrical current and operating environment on contact resistance and adhesion properties in order to correlate the resistance and adhesion behaviors with fundamental degradation mechanisms such as micro-welding, surface oxidation (kinetics), contamination build-up, and changes of contact material properties. Two approaches will be followed to understand the degradation mechanisms. In the first approach, different metal coatings will be developed using solid-state diffusion processes between multiple thin film layers. Annealing treatments and diffusion kinetics will be used to develop intermixed coatings having different compositions that provide a range of adhesion and contact resistance properties to uncover prevailing degradation mechanism(s). The second approach explores the contact resistance and adhesion properties of passivation layers and novel transfer coatings. Although less susceptible to micro-welding, the effects of surface asperities and organic contaminants on contact resistance will reveal potential degradation processes for these materials as MEMS contacts. A test methodology will be developed that evaluates fundamental coating properties followed as well as long-term coating performance, using a MEMS functionality test vehicle. Computational techniques will be explored with which to model the interactions at surface asperities. The purpose of this task is to understand the capabilities of numerical models to predict contact resistance and sticking properties versus surface asperities and material properties.

Keywords: MEMS, Dynamic Electrical Contacts

238. CONTROLLED FABRICATION OF NANOWIRE SENSORS
$435,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Francois Leonard, (925) 294-3511

We propose an integrated multi-disciplinary approach, from nanowire synthesis and device construction to theoretical modeling, in order to develop a new class of sensors with nanowires as the active elements. This new class of sensors is based on dramatic changes to nanowire conductivity when analytes interact with their surface, because of the high nanowire surface-to-volume ratio. This new class of sensors will address the needs of Homeland Security for ultra-sensitive detection, and our solution-based fabrication will allow for simple and inexpensive production. Synthetically, we will grow nanowires of different compositions, and will functionalize them with various organic functional groups, in order to tailor their response to specific agents. On the fabrication front, we will use advanced lithography combined with AC dielectrophoresis to place nanowires between electrodes and perform electrical measurements on these devices. We have done proof-of-principle experiments by fabricating carbon nanotube devices using this method, and have shown they have high sensitivity to chemicals. Our experimental efforts will be coupled with our first-principles modeling capabilities in quantum electronic transport. Such modeling will be necessary to understand the sensors to be built and to study the sensitivity of the nanowire conductivity to chemical, biological and optical stimuli. Given the expertise we have separately developed in synthesis, device fabrication and modeling, we propose to combine our efforts to produce a new class of sensors.

Keywords: Fabrication, Nanowires, Sensors

239. FUNDAMENTAL ENABLING ISSUES IN NANOTECHNOLOGY: STRESS AT THE ATOMIC LEVEL
$300,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Edmund Webb, (505) 284-6517

To effectively integrate nanotechnology into functional devices, fundamental aspects of material behavior at the nanometer scale must be understood. Stresses generated during thin film growth strongly influence component lifetime and performance; stress has also been proposed as a mechanism for stabilizing supported nanoscale structures. Yet the intrinsic connections between the evolving morphology of supported nanostructures and stress generation are still a matter of debate. We propose fully atomistic, coupled atomistic/continuum, and fully continuum simulations to predict stress generation mechanisms and magnitudes during all growth stages, from island nucleation to coalescence and film thickening. Simulations will be validated by electrodeposition growth experiments on patterned substrates, which can establish the dependence of microstructure and growth stresses on process conditions and deposition geometry. Deposition on nanopatterned substrates will permit stress measurements for isolated nanoislands. Sandia is one of the few facilities with the computational resources to attempt atomistic modeling of stress generation mechanisms during thin film growth. Fully atomistic simulations will explore surface stress induced pressure (Laplace pressure) for isolated nanoislands. Island coalescence stress for island radii up to 0.25 micron will be studied with atomic scale detail; results will reveal atomic structural changes associated with growth stress as a function of deposition conditions. A coupled atomistic/ continuum method will expand simulation length scales, permitting investigation of stress evolution during later growth stages, e.g. continual island coalescence and adatom incorporation into grain boundaries. The predictive capabilities of simulation permit direct determination of fundamental processes active in stress generation at the nanometer scale while connecting those processes to continuum models for much larger island and film structures. Our results will reveal the necessary materials science to tailor stress, and therefore performance, in nanostructures and, eventually, integrated nanocomponents.

Keywords: Nanostructures, Stress, Morphology

240. EFFECTIVE DISPERSION OF NANOPARTICLES BY POLYMERS
$200,000
DOE Contact: Mike Long, (202) 586-4595
SNL Contact: Dale Huber, (505) 844-9194

Polymeric materials filled with dispersed nanoparticles show great promise for lowering the thermal expansion coefficient in NW components and for use as high resolution photo-resists for lithography of novel microsystems. Also, the dispersion of nanoparticles is essential for a variety of other technologies important to Sandia, including high dielectric constant composites, ceramic processing, and solid-state lighting. However, materials processing is a critical issue: stable nanoparticle dispersions are difficult to achieve, as traditional colloidal techniques are not effective for nanoparticles. Steric stabilization by attaching macromolecules to the particles has been shown to work in specific cases, but the underlying science is not well understood. In order to determine the optimal way to disperse nanoparticles in silicones and other fluids, we will investigate the steric stabilization of nanoparticles by macromolecules. We will synthesize nanoparticles and attach polymers by functionalization or by polymerizing directly off the particle surfaces. We will explore the effectiveness of various surface coverages, molecular weights, and charges for dispersing nanoparticles. The experiments and characterization will provide input for and be interpreted using results from self-consistent field and classical density-functional theory. Theoretical work will include predicting the structure of the polymeric layers and the interaction energy between coated nanoparticles. The ultimate goal of this work is to enable the use of dispersed nanoparticles in nanocomposite materials for applications to NW components and microsystems, as well as other applications such as solid-state lighting and ceramics.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Keywords: Nanoparticles, Dispersion, Polymers

LAWRENCE LIVERMORE NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

241. ENGINEERED NANOSTRUCTURE LAMINATES
$6,200,000
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. These materials, while opening new approaches to solving problems of national security relevance, are now providing important scientific information and understanding relevant to the mechanical behavior of nanostructured materials.

Applications now under development include: IR, Visible, 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, lightweight optical systems.

Keywords: Precision Thin Films, Multilayer Nano-Laminate Technology, Energetic Materials, IR, Visible, UV, EUV, Soft X-Ray, X-Ray, Optics, Optical Systems, Advanced Joining Techniques, Rapid Manufacturing, Lightweight Space Optics, EUV Lithography, Energetic Structural Materials, Armor

242. AFM INVESTIGATIONS OF BIOMINERALIZATION
$200,000
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, X-ray absorption spectroscopy and optical spectroscopy to investigate the effects of small inorganic and organic growth modifiers, peptides, and proteins on the nucleation and growth of single crystals from solution. From these measurements we seek to determine growth mechanisms, stereochemical relationships, and the effect on the thermodynamic and kinetic parameters controlling orientation, morphology and growth rate.

Keywords: Biomineralization, Atomic Force Microscopy, Crystal Growth

243. BERYLLIUM ABLATOR COATINGS FOR NIF TARGETS
$1,400,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LLNL Contacts: Steve Letts, (925) 422-0937 and R. Wallace, (925) 423-7864

This program has as its objective the development of materials and processes that will allow sputter-deposition of up to 170 µm of a uniform, smooth, high-Z doped Be-based ablator on a spherical hollow mandrel. The work has been done in coordination with work at General Atomics in San Diego. 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 producing graded Cu-doped layers, developing laser drilling techniques that will be needed for capsule filling, and plastic mandrel removal via combustion through the drilled hole.

Keywords: Beryllium, Laser Fusion Targets, Ablator, Sputter Deposition

244. PLASMA POLYMER COATING TECHNOLOGY FOR ICF TARGETS
$300,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LLNL Contacts: 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 primary effort of the work has been shifted to General Atomics in San Diego. The approach involves first forming a symmetric 2-mm-diameter shell mandrel from poly(α-methylstyrene) by microencapsulation. This is then overcoated with a thin (12-15 µm) layer of CH plasma polymer formed by flowing a feed gas (CH_4 or C_4H_6,) plus H_2 through an R/F field to form molecular fragments which coat the shell in a bounce pan. Pyrolysis of the poly(α-methylstyrene) to gaseous monomer that diffuses away leaves the spherically symmetric, thermally stable CH shell behind. Additional coating to 150 µm gives a NIF capsule target. The focus in FY05 was in determining the oxidation rates of the plasma polymer material and in forming radial Ge-doped layers in the capsules.

Keywords: Polymers, Laser Fusion Targets, Plasma Polymer, Ablator

LOS ALAMOS NATIONAL LABORATORY

CAMPAIGN 8 AND THE JOINT MUNITIONS PROGRAM (DOD/DOE)

245. ENHANCED SURVEILLANCE OF HIGH EXPLOSIVES
$3,070,000
DOE Contact: Eric Cochran
LANL Contact: Sheldon Larson, (505) 667-7854

Stockpile stewardship constitutes the core mission of the Department of Energy's National Laboratories. At the heart of stockpile stewardship, the Enhanced Surveillance Campaign is tasked with one of the most difficult technical challenges ever faced. The goal of the High Explosives (HE) MTE is to determine if and when age-related changes in explosive components (main charge, boosters, detonator and actuators) begin to affect weapon performance or safety. The HE MTE helps assess the current health of nuclear weapons and predicts HE component behavior as these parts age beyond their intended lifetime. The Enhanced Surveillance Campaign will provide age-related, science-based predictions of changes in HE performance and safety so that designers can improve large-scale, 3-D simulations with more rigorous estimates of levels of accuracy, limits of applicability, and degrees of confidence. These simulations, however, require validation, and ESC will also obtain experimental data and develop diagnostics to measure new data that will test the physics and engineering models.

FY05 Efforts: High explosive components must function adequately in terms of performance, safety, and structure. Of these three categories, HE performance is the most straight forward property to assess because current weapon applications contain variable inputs for values such as detonation velocity and product equation of state (EOS). Past efforts evaluated the performance of PBX 9501, but to date, no degradation in performance has been observed. In FY05, we continued to evaluate the performance of naturally-aged PBX 9502 through measuring initiation and run-up to detonation. PBX 9502 is less robust than PBX 9501 and subtle changes in performance may significantly alter the performance of a weapon. Before we can attribute changes due to age, however, variation due to lot-to-lot differences and virgin versus 50% recycled material must be measured. Work in collaboration with Honeywell KCP seeks to improve resolution through hardware and software development. Additionally, we are developing a failure cone diagnostic for measuring the detonation behavior of PBX 9502. Core surveillance does not include routine testing of PBX 9502 performance, something desired by LANL HE scientists. Efforts to search for possible changes in PBX 9502 performance with age will help lifetime assessments and annual certification input for the B61 main charge.

Performance is not the only factor that could limit the service life of HE. Weapons must maintain their designed safety in all handling, storage, and transportation scenarios. Explosive safety, as measured in terms of sensitivity, is much more difficult to assess than performance. The sensitivity of an explosive is not a well-defined property. Sensitivity is a complex pattern of behavior that depends, for one, on the type of stimulus. Whereas the performance of HE depends on its behavior when intentionally initiated by a shock wave, HE can be unintentionally initiated by many different stimuli, such as, friction, heat and various types of impact. Explosives in nuclear weapons are desensitized by formulating with plastic binders (PBX 9501 & PBX 9407 for example). As the binder degrades, the explosive sensitivity is likely adversely effected. In FY05, we continue to evaluate the sensitivity of artificially-aged PBX 9501. The modified Steven tests are only one configuration of sensitivity test. Modelers, however, consider this an important diagnostic for gaining insight into shear forces leading to fracture and ignition. An extensive effort is underway to describe experimental results and the developed models will be eventually incorporated in engineering safety codes.

A second sensitivity test has been under development in collaboration with Pantex for several years. This effort seeks to measure possible changes in output of the XTX 8004 component. The function of XTX 8004 components and age-related changes are concerns of physics safety designers and outside oversight agencies, such as the DNFSB. The high priority of the development of this diagnostic is an indication of the emphasis on safety within ESC activities. This milestone was achieved in FY05, and the XTX 8004 safety/function test is ready for deployment in core surveillance.

Since its inception, the HE MTE has been focused primarily on the degradation of the PBX 9501 binder. The reason for this emphasis is twofold. First, PBX 9501 is used as a maincharge explosive in several weapon systems and upcoming LEPs need to determine future replacement of this commonly used HE. Second, PBX 9501 is known to age through chemical reactions of the polymer binder, and therefore, understanding the aging is critically important in assessing its service life. A significant effort is continuing in FY05 to identify the reaction mechanisms responsible for binder degradation. Strong collaboration with scientists at Pantex exist and several aging studies at both LANL and PX are ongoing. Spectroscopic techniques, such as Small-angle scattering (SAS), NMR, GC/MS, HPLC continue to be used to help unravel aging chemistry. In FY05, we will continue to exploit isotopic labeling of model compounds in order to probe reaction chemistry using SAS and NMR. Previous work in describing the hydrolysis of Estane is nearly completed. Hydrolysis alone, however, does not adequately account for the observed degradation of the binder, and emphasis has shifted to examining oxidation mechanisms involving free radicals. The complex role of the stabilizers (Irganox or DPA) and nitroplasticizer is beginning to be unraveled by ESC scientists.

Estane degradation in PBX 9501 will ultimately affect the mechanical integrity of the HE charge and impact the weapon reliability. Linking chemical degradation to mechanical properties is an ongoing effort in ESC. Added to the complexity is that Estane is a block co-polymer consisting of “hard” and “soft” domains. Understanding how these domains behave within the HE composite during aging is key to understanding how changes in chemistry influence the mechanical behavior. The HE MTE employs several sophisticated techniques to probe the chemical and physical properties of the binder during accelerated and naturally aged experiments. In FY05, we continued the development of a micro-mechanical strength model that will link chemical changes in Estane to mechanical properties of Estane and the HE composite.

All activities, experimental studies investigating reaction chemistry of the binder, mechanical and fracture studies to characterize HE behavior, and model development that describe aging properties and link these to weapon codes are vital for providing updated lifetime assessment of PBX 9501.

Keywords: High Explosives, Aging, Degradation

246. MIC PROJECT
$389,000
NNSA Contact: Bharat Agrawal, (301) 903-2057
LANL Contact: Tim Foley, (505) 665-3583

This project focuses on using advances in the control of particle sizes down to the nanometer level to generate new and novel behavior from conventional energetic systems. Systems similar to traditional thermites have been examined and it has been demonstrated that by changing the particle size and identity of the constituents, materials can be made that act as primary or secondary explosives or to burn like propellants. Materials can have propagation rates that can range from cm/s to km/s, have pressure outputs the range from 10 psi/mg to none at all and can have densities greater than 6 g/cc. By defining the parameters that determine the behavior of these systems, energetic composites can be produced whose properties are engineered to any application. Currently, these materials are being evaluated as replacements in percussion primers for small and medium caliber munitions, actuating charges and ignition delays. A highlight for FY 05 was the development of a system that had a steady-state propagation velocity of 2.5 km/s.

Keywords: Energetic Materials, Composites, Nanoparticles

247. HIGH EXPLOSIVE CRYSTAL GROWTH AND CHARACTERIZATION
$225,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LANL Contact: Dan Hooks, (505) 667-6407

This project is jointly supported by the Office of Naval Research and the DOE/DOD Joint Munitions Program. The goals are to grow, prepare samples from, and characterize single crystals of molecular explosives. The characterization work is done collaboratively with many groups at LANL, in addition to several DOE, DOD, and University Laboratories. The characterization work is performed to understand the basic properties of the materials to help build constitutive material models for complex plastic bonded explosives, and to unravel the complex pathways leading to detonation. The laboratory is unique in the country because very large (>50g) single crystals can be prepared. These large crystals are sometimes required to prepare samples for certain experiments. Major accomplishments in FY05 include characterization of defects in crystals, the first small scale laser shock experiments, a study of the Hugoniot elastic limit of RDX, continuing work on the shock initiation of HMX, and isentropic compression of HMX and plastic bonded explosive constituents.

Keywords: Energetic Materials, Constitutive Models, Plastic Explosives

248. DAMAGE IN MOCK EXPLOSIVE MATERIALS
$75,000
DOE Contact: Robert Hanrahan, (202) 586-4606
LANL Contact: Carl Cady, (505) 667-6369

The goal of this project in FY05 was to evaluate damage imparted into a mock 900-21 charge that was part of a full assembly subjected to a load. The evaluation was compared with predictions calculated using visco-SCRAM. Full details are classified.

Keywords: Explosives, Damage

249. SHOCK INITIATION EXPERIMENTS ON THE TATB BASED EXPLOSIVE PBX 9502: COMPARISON OF BASELINE AND AGED MATERIALS
$375,000
DOE Contact: Robert Hanrahan, (202) 586-4606
LANL Contact: Rick Gustavsen, (505) 667-2086

We have completed a series of ambient temperature (23 ±2˚C) shock initiation experiments on four lots (batches) of the insensitivehigh explosive PBX 9502. PBX 9502 consists by weight of 95% dry-aminatedTri-Amino-Tri-nitro-Benzene (TATB) and 5% of the plastic binder Kel-F-800, a 3/1 co-polymer of chloro-trifluoro-ethylene and vinylidene-fluoride. Twoof the 4 lots were manufactured using the “Virgin” process. Both of these lots had few fine TATB particles. One Virgin lot was stored the majority of its life (>15 years) as molding powder and pressed as a 240 mm diameter by 130 mm thick cylinder. The other Virgin lot was stored the majority of its life as a hollow hemispherical pressing. Two lots were manufactured using the “Recycle” process and had many fine TATB particles. One “Recycled” lot was stored the majority of its life as molding powder while the other was stored as a pressed charge. Shock initiation experiments were performed using precisely characterized planar shocks generated by impacting an explosive sample with a projectile accelerated in a two-stage gas gun. Evolution of the shock into a detonation was measured using ten or eleven embedded electromagnetic particle velocity gauges and three “shock tracker” gauges. Results include: 1) high quality particle velocity waveforms which should be useful for calibrating reactive burn models, 2) no difference in sustained shock initiation response between lots regardless of material processing or storage history, 3) response for all lots equivalent to that measured by Dick, et al., 4) additional Hugoniot and Pop–plot data for PBX 9502, 5) short shock response which, when compared to the sustained shock response, shows no extension in run distance unless the rarefaction overtakes the shock front prior to the distance it would have run to detonation as a sustained shock.

Keywords: Energetic Materials, Shock Initiation, Aging

250. DYNAMIC BEHAVIOR OF POLYMERS AND FOAMS
$625,000
DOE Contact: Robert Hanrahan, (202) 586-4606
LANL Contact: Dana M. Dattelbaum, (505) 667-7329

Polymer and foam materials are pervasive in both our conventional and nuclear weapons. Experimental data to support the construction and validation of theoretical models to describe polymer behavior under quasi-static to dynamic loading conditions is lacking for many materials of interest to DOE. Both engineering models and equations-of-state are required to describe polymer behavior in weapons applications. This program aims to address our current deficiencies through a coupled experimental and theoretical effort. Activities include chemical analysis (thermal analysis, spectroscopy, chromatography), quasi-static to intermediate rate mechanical property testing, dynamic plate impact experiments (shock), high pressure diamond anvil cell experiments, chemical decomposition experiments to identify products (detonation chemistry apparatus), and development and investigation of model materials to understand polymer network behavior. For each experimental activity, there is a complimentary theoretical effort, including constitutive model development, reactant and product equation-of-state, molecular dynamics simulations, and micro-mechanical simulations. Highlights for fiscal year 2005 include a first baseline equation-of-state and measurement of mechanical properties for cross-linked poly(dimethylsiloxane) (PDMS) foams of interest, and a filled polymeric composite, measurement of absolute heat capacities, simulation of open cell foams and preliminary simulations of closed cell foams under compression, development of a quantum chemical potential for PDMS, comparison of mechanical properties of new vs. aged materials, and the development of constitutive models with importation of data into a new Laboratory materials database.

Keywords: Equation-of-State, Polymers, Composites, Mechanical Properties, Shockwave Physics

251. EXPLOSIVES CHEMISTRY AND PROPERTIES
$501,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LANL Contact: David E. Chavez, (505) 665-2742

The goal of the Explosives Chemistry and Properties project is to prepare, characterize, scale-up and study new energetic materials to provide broader weapons design capabilities. To achieve this goal six objectives are being pursued: 1) increase the energy (by 10% over HMX or 80% of HMX for insensitive munitions) through increases in density or improvements in thermochemistry (DH_r, DH_f); 2) Improve propellant performance compared to TAGZT (increased energy, reduced impact, friction sensitivity, improved morphology); 3) maintain or improve the impact and shock sensitivity by 25% over HMX (or explosive D for insensitive munitions), 4) add chemical intelligence to HE chemistry database, 5) improve existing kinetics models for burn-rate behavior of high-nitrogen materials Highlighted below are two examples of accomplishments in FY06 that demonstrate progress towards achieving these goals. FY05 Highlights include: Several high-nitrogen transition metal complexes were identified and potential replacements for lead azide/lead styphnate primary explosive applications and full characterization is ongoing. A related high-nitrogen metal complex project received an R&D 100 award in FY 2005. Work in the area of high-nitrogen materials continued with the highlight of exclusive licensing of BTATz for inflation safety devices by a domestic commercial partner.

Keywords: Energetic Materials, Chemistry Database, Kinetic Models

252. MICROSTRUCTURAL AND KINETIC EFFECTS ON THE BEHAVIOR OF ENERGETIC MATERIALS
$950,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LANL Contact: Bryan Henson, (505) 665-4837

This is a fundamental research project within the Los Alamos Joint Munitions Program with the goal of understanding the mechanisms of energetic material response and applying this understanding toward improving the safety of CHE and the performance of IHE explosives. Our approach involves the development and application of small scale experiments which allow the interrogation of processes ranging from the response of a material to heating, thermal runaway and ignition, the subsequent propagation of ignition by convective or conductive burning, transition to detonation, and full scale detonation performance and sensitivity. We apply this suite of experiments to three main tasks in the project. In the first task we use small scale laboratory experiments and larger, integral thermal explosion experiments to generate data for the validation of multi-step kinetic decomposition models, ignition mechanisms and combustion propagation models. In the second task we are developing and validating small scale detonation sensitivity and performance experiments. These experiments are used to generate mechanisms of weak shock propagation, ramp wave desensitization and detonation energy release. In the third task we investigate new material morphologies and mixtures which reflect understanding gained from the first task. We validate the expected behavior of these new materials using the experimental techniques developed in tasks one and two.

Keywords: Energetic Materials, Microstructure, Kinetic Models

253. PROTON RADIOGRAPHY OF A THERMAL EXPLOSION IN PBX 9501
$600,000
DOE Contact: Robert Hanrahan, (202) 586-4606
LANL Contact: Laura Smilowitz, (505) 667-5207

This is a fundamental research project within the Los Alamos Science Campaigns 1 and 2 with the goal of understanding thermal ignition and the propagation of energy release in PBX 9501. The understanding of thermal explosions has been hindered compared to that of detonations by the difficulty of predicting the exact time of the event. A radiographic technique such as proton radiography can illuminate the events at the center of a thermal explosion, but requires the ability to control ignition time to within a hundred microseconds. We have developed a technique for synchronizing a thermal explosion at the center of a heated explosive with hundred microsecond accuracy. Synchronization is achieved by using a fiber coupled laser to provide a temperature perturbation within the ignition volume. Using a convergent heating geometry and carefully chosen heat profile to determine the ignition location and then synchronizing the ignition to the LANSCE proton accelerator at Los Alamos we demonstrated the first such radiographic experiments in November, 2005. The images obtained give us the first measure of mass loss during thermal decomposition at the center of a heated explosive. The dynamic images at ignition reveal the ignition of burning and consumption of energetic material and are being used to develop a model for burn propagation which includes cracking, convection, and conductive consumption of material. Continued experiments will allow us to better understand thermal explosion phenomena and will open up the field of thermal explosion research to diagnostics previously inaccessible.

Keywords: Energetic Materials, Proton Radiography, Burn Propagation Model

254. THERMAL RESPONSE OF PBX 9501
$300,000
DOE Contact: Bob Jones
LANL Contact: Bryan Henson, (505) 665-4837

This work is part of a project within the Los Alamos Surety and L.E.P. programs whose overall motivation is predicting the outcome of an accident or threat scenario which involves the heating of PBX 9501 either by direct means or through impact. Understanding this thermal response of PBX 9501 is critical to weapons safety and surety issues. The response is a very complex function of the temperature, which depends upon the mechanism of heating. We apply a suite of experiments to heat small, intermediate and large scale samples of PBX 9501. In small scale experiments we examine the fundamental mechanisms of material damage as a function of temperature and chemical decomposition. In intermediate scale experiments we apply these fundamental models to thermal explosion tests conducted either by direct or impact induced heating. At the large scale we validate the models against observed response in large tests conducted at outdoor firing sites. Considerable new understanding of thermal response in this material has resulted from these studies, including the fact that a single model of thermal response can be used to model ignition in all plausible heating scenarios, and that measurements of internal ignition can be used to understand not only the ignition mechanism but the subsequent release of energy in an explosion. These observations relate directly to understanding the thermal response of PBX 9501 to a variety of safety and threat scenarios.

Keywords: Energetic Materials, Thermal Response

255. JMP: POLYMER BEHAVIOR UNDER DYNAMIC LOADING
$1,000,000 (joint DOE and DoD contribution)
DOE Contact: Bharat Agrawal, (301) 903-2057
LANL Contact: B. E. Clements, (505) 667-8836

This project has as its objective the development of high-precision physics-based theoretical constitutive models to be used in engineering simulation and design. An associated objective is to populate materials databases with experimental data necessary for polymer constitutive model generation and validation. We have successfully investigated the polymers: Kel-F 800, used as a binder in the DOE high explosive PBX-9502; (poly)tetrafluoroethylene, used as a DoD reactive material matrix; (poly)etheretherketone, used as a DOE structural polymer; polycarbonate used for DoD face shields; and graphite-epoxy composites, used as DOE structural materials and DoD rocket casing materials.

Keywords: Energetic Materials, Polymers, Constitutive Models

256. THERMAL AND LOADING DYNAMICS OF ENERGETIC MATERIALS
$1,250,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LANL Contacts: Cheng Liu, (505) 665-6892 and Sherri Bingert, (505) 667-7615

The safety of nuclear weapons is of the utmost importance to the Department of Energy, and the high explosives that initiate a weapon have been the most vulnerable component in the system. Similarly, the survivability of the high explosives during the process of launch, flight, impact, and penetration is of great concern to the Department of Defense, because it will affect the performance and lethality of a weapon system. In the meantime, accurate and adequate assessment of response of the solid propellant and high explosives are lying at the core of the insensitive munitions (IM) technologies and will impact the IM compliance of many systems. As a result, properties and performance of energetic materials during non-shock processes and under abnormal conditions have become urgent and important issues.

The goals of this project are the following: develop physics-based high explosive constitutive models; establish experimental data bases that cover wide range of strain rates and temperatures; develop computer codes and implement the models into computer codes so we can predict HE response under the abnormal, non-shock loading conditions; accumulate comprehensive test cases for validating HE constitutive models, and transfer the models to both DoD and DOE customers.

Keywords: Energetic Materials, Constitutive Models, Mechanical Characterization

OFFICE OF FOSSIL ENERGY

	FY 2005
OFFICE OF FOSSIL ENERGY GRAND TOTAL	$12,543,000
OFFICE OF ADVANCED RESEARCH	$12,543,000
ADVANCED RESEARCH MATERIALS PROGRAM	$6,978,000
PROGRAM OVERSIGHT AND COMMUNICATIONS	$470,000
Management of the Advanced Research Materials Program	430,000
Personal Services Contract	15,000
Materials and Components in Fossil Energy Applications Newsletter (MCNL-5)	25,000
NEW ALLOYS	$2,713,000
Materials for Ultra-Supercritical Steam Power Plants (FEAA061)	860,000
Ultra-Supercritical Steam Cycle Turbine Materials (FEAA069)	450,000
Steam Turbine Materials and Corrosion (ARC-2)	200,000
Advanced Pressure-Boundary Materials (ORNL-2C)	240,000
Continuation of Studies on Development of ODS Heat Exchanger Tubing (FEAA058)	173,000
Enabling the Practical Application of Oxide Dispersion-Strengthened Ferritic Steels (ORNL-2E)	210,000
ODS-Alloy Development for High Temperature Heat Exchangers (UCSD-2)	125,000
Reduction in Defect Content in Oxide Dispersion-Strengthened Alloys (UL-2)	150,000
Testing of a Very High-Temperature Heat Exchanger for IFCC Power Systems (UNDEERC-4)	55,000
Fireside and Steamside Corrosion of Alloys for USC Plants (ANL-4)	175,000
In-Plant Corrosion Probe Tests (FW-5)	75,000
COATINGS	$1,285,000
Extended-lifetime Metallic Alloys and Coatings for High-Temperature Environmental Protection (ORNL-2B)	220,000
High-Temperature Corrosion Resistance of Fe-Al-Cr Weld Overlay Coatings (LU-2)	120,000
Chemically Vapor Deposited YSZ for Thermal and Environmental Barrier Coatings (ORNL-1A)	225,000
Modeling of Chemical Vapor-Deposited Zirconia for Thermal Barrier and Environmental Barrier Coatings (UOL-3)	65,000
Aluminide Coatings for Power-Generation Applications (TTU-2)	70,000
Influence of Processing on Coating Microstructure and Properties (INEL-2)	170,000
Corrosion Resistant Ceramic Coatings (ORNL-1B)	200,000
Development of Nondestructive Evaluation Methods for Ceramic Coatings (ANL-1)	215,000
FUNCTIONAL MATERIALS	$1,460,000
Low-Chrome/Chrome Free Refractories for Slagging Gasifiers (ARC-1)	200,000
Development of Novel Activated Carbon Composites (ORNL-3E)	330,000
Development of Inorganic Membranes for Hydrogen Separation (ORNL-3B)	245,000
The Production of Pure Hydrogen from Hydrocarbons (LANL-3)	100,000
Gas Sensors for Fossil Energy Applications (ORNL-3H)	235,000
Sealing Technology for Gas Separation Membranes (PNL-3)	350,000

OFFICE OF FOSSIL ENERGY (cont.)

	FY 2005
OFFICE OF ADVANCED RESEARCH (cont.)	
ADVANCED RESEARCH MATERIALS PROGRAM (cont.)	
BREAKTHROUGH CONCEPTS	$1,050,000
Multi-Phase, High-Temperature Alloys: Exploration of Laves-Phase Strengthened Steels (ORNL-2D)	110,000
Mo-Si-B Alloy Development (ORNL-2I)	140,000
Influence of Impurities on Ductility of Cr- and Mo-based Alloys and In-Situ Mechanical Property Measurement (WVU-2)	140,000
Novel Processing of Mo-Si-B Intermetallics for Improved Efficiency of Power Systems (AMES-2)	75,000
Study of Fatigue and Fracture Behavior of Ti-Al-Nb-W-B Intermetallic Materials (UT-2A)	95,000
Novel Structures and Properties Through Controlled Oxidation (ORNL-4A)	200,000
Concepts for Smart, Protective, High-Temperature Coatings (ORNL-4C)	120,000
Pilot Facility for the Production of Silicon Carbide Fibrils (REMAXCO-5)	100,000
Advanced Processing of Metallic Powders (AMES-3)	70,000
ADVANCED METALLURGICAL PROCESSES PROGRAM	$5,565,000
MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING	$915,000
Advanced Casting Technologies	400,000
Effect of Reactive Element Surface Infusion on the Oxidation Behavior of Alloys	200,000
High Temperature Strengthening Concepts in High Performance Materials for Energy Applications	315,000
MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING	$4,650,000
Advanced Refractories for Slagging Gasifiers	600,000
Low-Chrome/Chrome Free Refractories for Slagging Gasifiers	500,000
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	1,000,000
Materials Performance for Heat Exchangers & Other Balance of Plant Components for Solid Oxide Fuel Cells	1,000,000

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, ORNL has the responsibility of the technical management and implementation of all activities in 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

257. MANAGEMENT OF THE ADVANCED RESEARCH MATERIALS PROGRAM
$430,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins, (865) 576-4507
ORNL 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 maintaining awareness of related developments and key programs being conducted elsewhere; recommending work to be accomplished by subcontractors, other federal laboratories, and by ORNL; preparing its budget proposals (FWPs) for the program; 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, NETL

258. PERSONAL SERVICES CONTRACT
$15,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins, (865) 576-4507
ORNL 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

259. MATERIALS AND COMPONENTS IN FOSSIL ENERGY APPLICATIONS NEWSLETTER (MCNL-5)
$25,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
ORNL 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

260. MATERIALS FOR ULTRA-SUPERCRITICAL STEAM POWER PLANTS (FEAA061)
$860,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins (865) 576-4507
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The purpose of this 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 of 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 essentially no experience in steam plant. The research undertaken here is in direct support of the US USC Steam Tubing Consortium program (that involves all of the domestic boiler makers), and is generating data and understanding that will provide an essential database to the designers, manufacturers, and users of the USC steam plant.

Keywords: Ultra-Supercritical, Boiler, Ni-based Alloys

261. ULTRA-SUPERCRITICAL STEAM CYCLE TURBINE MATERIALS (FEAA069)
$450,000
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Current state-of-the-art coal-fired supercritical steam power plants operate with high-pressure turbine inlet steam temperatures close to 600°C. The best of the recently-developed and commercialized advanced 9-12Cr martensitic-ferritic steels may allow prolonged use at temperatures to about 620°C, this is probably close to the inherent upper temperature limit of such steels. Further increase in the temperature capability of advanced steam turbines will require the use of Ni-based superalloys and system redesign, as is being pursued in several European and Japanese programs that are pioneering advanced power plants capable of operating with steam up to 700°C. This effort complements the US USC steam program to qualify boiler tubing and piping alloys for use up to 720/760°C, and is aimed at the development of the enabling materials for the corresponding USC steam turbine. The research undertaken here is in direct support of the US USC Steam Turbine Consortium program (that involves all three domestic steam turbine manufacturers), and provides expertize and capabilities that are not available at any single manufacturer. The efforts have addressed an expanded portfolio of alloys that includes cast austenitic stainless steels and alloys, in addition to various Ni-based superalloys for critical turbine components. Preliminary input from utilities indicates that cost-effective improvements in performance and efficiency that do not sacrifice durability and reliability are prime considerations for any advanced steam turbine technology.

Keywords: Ultra-Supercritical, Turbine, Stainless Steel, Alloy

262. STEAM TURBINE MATERIALS AND CORROSION (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
National Energy Technology Laboratory, Albany Contact: G. R. Holcomb, (541) 967-5874

Advanced or 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 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 systems, with emphasis placed on alloys for high- and intermediate-pressure turbine sections. Strength requirements at temperatures as high as 760˚C have led to most of the efforts being directed to nickel-base alloys containing chromium. This project has or will examine the effects of temperature, pressure and specimen geometry on oxidation resistance using a variety of exposure tests and post-test measurements and examinations.

Keywords: Ultra-Supercritical, Steam-Side Oxidation, Alloys, Chromium

263. ADVANCED PRESSURE-BOUNDARY MATERIALS (ORNL-2C)
$240,000
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ORNL Contact: J. P. Shingledecker, (865) 574-5108

The purpose of this task is to evaluate the processing-structure-property relationships in high-temperature structural alloys to optimize their use for components in advanced, combined-cycle, and coal-combustion systems, with emphasis on cycles aimed at operating at temperatures of 700ºC and higher. One group of alloys with the potential to satisfy the conditions required of higher operating temperatures is the advanced ferritic steels, such as P91, P92, and P122. These are Cr-Mo steels containing 9-12 wt% Cr that have martensitic microstructures. Research aimed at increasing the operating temperature limits of the 9-12 wt% Cr steels and optimizing them for specific power plant applications has been actively pursued since the 1970's. One of the newer class of 12 wt% Cr steels is SAVE12 which is alloyed with significant amounts of cobalt and tungsten. Creep test data indicate that SAVE 12 may be suitable for service up to 650˚C, making it an especially attractive alloy. As with all of the high strength martensitic steels, specifying upper temperature limits for tempering the alloys and heat treating weldments is a critical issue. To support this aspect of development, thermodynamic analysis was used to estimate how this critical temperature, the A_1 in steel terminology, varied with alloy composition. The results from the thermodynamic analysis were then used to construct a simple PC-based application program to estimate A_1. The computer application will be demonstrated.

Recent studies at the Steel Research Center of the National Institute for Materials Science (NIMS) in Japan indicate that Type IV cracking at welds can be eliminated by alloying 9Cr steels with relatively high concentrations of B, and low concentrations of N. The reasons for this unusual and potentially significant behavior are unclear, but they appear related to the nucleation and growth of austenite during heating and cooling cycles in weld heat-affected zones. One possibility is that the B addition suppresses austenite nucleation and growth during heat-affected zone thermal cycles. A second possible mechanism is that the base metal contains retained austenite which is distributed so that the original coarse austenite grain size is regenerated during heat-affected zone thermal cycles. To date, however, efforts to identify retained austenite in the base metal microstructure have been inconclusive. In collaboration with NIMS staff, diffraction experiments were conducted at the Advanced Photon Source, Argonne National Laboratory, to determine the transformation behavior of their experimental steel and P92 steel under simulated weld heat-affected zone thermal cycles. The value of this approach will be critically assessed and, if its initial promise is confirmed, it will be used in further efforts for elucidating routes for improving alloy strength at temperature.

Keywords: Alloys, Combined-Cycle, Chromium, Tungsten

264. CONTINUATION OF STUDIES ON DEVELOPMENT OF ODS HEAT EXCHANGER TUBING (FEAA058)
$173,000
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This project is intended to generate information and understanding for incorporation into a database being generated by a 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. 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. The effort at ORNL has the objectives of: 1) extension of a transient liquid-phase bonding technique for use with ODS-FeCrAl alloys (in conjunction with an external consultant, and with J.P. Hurly at UNDEERC); 2) elevated-temperature mechanical testing of joints, to evaluate the effect of joining on high-temperature, oxidation-limited, service life of the tubes; and 3) assembly of data required by designers, and review of implications of ODS properties on heat exchanger design. Effort so far has concentrated on applying a transient liquid-phase bonding technique to butt-joints in the ODS-FeCrAl alloys MA956 and PM2000. Joints have been made that appear clean in transmission-electron microscopy, but the issue of redistribution of the Y-containing oxides in the vicinity of the bond has required several iterations of processing parameters. The desired result from such joining is that the alloy can be recrystallized to form the large grain structure needed for high-temperature creep strength, with no major disruption of the final microstructure around the joint. This leads to the concern that changes in the distribution and/or particle size of the yttria dispersoid may have a detrimental influence on the alloy recrystallization behavior. Implications from current studies are that the joining conditions used initially resulted in the presence of too much molten phase being present for too long, leading to some agglomeration of the dispersoid. Current iterations are based on routes to remedy these shortcomings.

Keywords: Alloys, ODS, EWI, Joining

265. ENABLING THE PRACTICAL APPLICATION OF OXIDE DISPERSION-STRENGTHENED FERRITIC STEELS (ORNL-2E)
$210,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
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Oxide dispersion-strengthened (ODS) ferritic steels are capable of developing creep strength at temperatures well in excess of those attainable by conventional alloys, and also possess exceptional environmental resistance. Currently, these alloys are not widely used because they are: 1) difficult to join, 2) very expensive, and 3) have unusual mechanical behavior (anisotropic properties). The overall goal of this project is to facilitate the exploitation of ODS alloys by addressing these perceived barriers, as well as to develop a mathematical model of the oxidation behavior to allow lifetime prediction; cost is considered to be an issue that will be resolved when these alloys are more widely used. Joining studies have concentrated on butt joints, using a pulsed plasma-assisted diffusion process developed by a small business via an SBIR grant. Bonds made in 19 mm rods of unrecrystallized ODS-FeCrAl were found by TEM to be microscopically clean, with only occasional particles of Al_2O_3 and Al_2O_3-TiC at the bond line. A creep-screening test at 900˚C indicated promising strength, with the strongest joint exhibiting 64% of the axial strength of the base alloy (and 188% the transverse strength). A further iteration of the most promising joining parameters has resulted in joints that offered little resistance to secondary recrystallization, so that the microstructure of the final joint was not interrupted in the vicinity of the bond. These joints are to be creep tested at 1000˚C to quantify any strength improvements. Hot torsion processing is being investigated as a route for improving creep strength of tubes in the hoop direction, and so reduce anisotropy. The recrystallized microstructure of 25 mm OD tubes processed to different angles of twist exhibited spirally-oriented grains with a (desired) reduction in length-to-width ratio (compared to the as extruded microstructure), and these are being evaluated to determine changes in creep strength at 1000˚C. In terms of oxidation lifetime model development, a relatively simple (though, mechanism-based) model based on consumption of Al has been demonstrated to give good agreement between observed and calculated values of time to onset of breakaway oxidation, over the temperature range 1000-1300˚C. Refinements needed include improved values for the minimum Al level at which breakaway oxidation ensues, as a function of temperature, and the incorporation of approaches to account for the development of Al concentration gradients, which vary with assumed component shape.

Keywords: Alloys, ODS, High Temperature, Joining, Oxidation

266. ODS-ALLOY DEVELOPMENT FOR HIGH TEMPERATURE HEAT EXCHANGERS (UCSD-2)
$125,000
DOE Contacts: F. M. Glaser, (301) 903-2784,
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University of California at San Diego Contact:
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The objectives of this program are to enhance high-temperature hoop creep-strength in ODS-alloy tubes and liner components and preferential cross-rolling, flow-forming and grain/particle fibering in the critical hoop direction. Recent studies of cross-rolled and flow-formed ODS-alloy tubes indicate that transverse creep was significantly enhanced by controlled transverse grain fibering and grain coarsening. This program systematically examines post-extrusion forming methodologies to create hoop-strengthened tubes, and evaluates such modifications at 'in-service' loads at service temperatures and environments. Furthermore, with a view to ultimately developing components and subsystems, efforts are also directed to evaluate kinetically-driven (inertia, magnetic pulse, and flash-upset welding) non-fusion joining processes. Three separate processes—inertia welding, magnetic-pulse welding and flash-upset welding—are deemed viable, as demonstrated by a series of butt- and lap-joint configurations in ODS alloy tubes in the current program.

Keywords: ODS, Joining, Alloys, Creep

267. REDUCTION IN DEFECT CONTENT IN OXIDE DISPERSION-STRENGTHENED ALLOYS (UL-2)
$150,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins , (865) 576-4507
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The University of Liverpool Contact: A. R. Jones, 151-794-8026

The high-temperature creep strength of the 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 and 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 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 being that the ODS-free regions in the alloy should provide sites for rapid re-crystallization 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, Modeling

268. TESTING OF A VERY HIGH-TEMPERATURE HEAT EXCHANGER FOR IFCC POWER SYSTEMS (UNDEERC-4)
$55,000
DOE Contacts: F. M. Glaser, (301) 903-2784, V. U. S. Rao (412) 386-4743, M. H. Rawlins, (865) 576-4507
ORNL 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 the coal in such an oxygen-blown system, the need for flue gas recirculation to manage the flame temperature is reduced and the 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.

The calculations show 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, whereas the operation of an IFCC is much better understood since it is essentially the same as current pc-fired systems. In addition, the results from flowing slag corrosion tests of 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 the switch grass blend because the solidus temperature of the slag was exceeded.

Keywords: High Temperature, Heat Exchanger, Combined Cycle

269. FIRESIDE AND STEAMSIDE CORROSION OF ALLOYS FOR USC PLANTS (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
ORNL Contact: I. G. Wright, (865) 574-4451
Argonne National Laboratory Contact: K. Natesan, (630) 252-5103

The objective of the present work is to evaluate the corrosion performance in coal ash, alkali sulfate, and alkali chloride environments of candidate materials for USC steam systems, with emphasis on temperatures in the range of 650-800˚C. The experimental program is aimed at developing a scientific understanding of corrosion mechanisms as a function of alloy composition and deposit chemistry, and at quantitatively determining the scaling, internal penetration, and metal wastage of the alloys. The project also involves corrosion evaluation of candidate alloys in steam environment at 650 to 800˚C. In addition, surface modification (via coatings) of alloys to improve the corrosion resistance is being explored. The current project has developed a significant amount of corrosion information and has also identified key process variables and alloy chemistry that need further study. The current project conducted primarily in a well-controlled laboratory environment is complementary to the program on boiler materials being conducted (via power-plant exposures) by the US USC Steam Tube industry consortium.

Keywords: Alloys, Corrosion, Ultra-Supercritical

270. IN-PLANT CORROSION PROBE TESTS (FW-5)
$75,000
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This project is designed to generate fireside corrosion data in actual coal-fired operation for the advanced, alloys that are candidates for application for the highest-temperature duty in heat transfer applications in DOE's advanced power systems. In-plant corrosion probes (made of ring sections cut from tubes) will be installed in a utility boiler and exposed at controlled metal temperatures up to 1093°C (2000°F). The primary objective is to assess the resistance to corrosion under conditions where deposits can form that are capable of developing molten phases, which are known to create the most aggressive environment for conventional alloys. The probes will be fabricated from oxide-dispersion-strengthened alloys MA956 and PM2000, and nickel-based superalloys, such as 230, 617, 693, 601, and 602CA.

Keywords: Alloys, ODS, Austenitic, Corrosion

COATINGS

271. EXTENDED-LIFETIME METALLIC ALLOYS AND COATINGS FOR HIGH-TEMPERATURE ENVIRONMENTAL PROTECTION (ORNL-2B)
$220,000
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The purpose of this task is to examine important composition and microstructure issues associated with the development of extended-lifetime corrosion-resistant metallic alloys and coatings for high-temperature applications associated with the key technologies of the Office of Fossil Energy's advanced power systems. The goal is to understand critical mechanisms for developing more oxidation-resistant alloys and coatings that form external, protective alumina layers or scales. For coatings, this program is focused on developing a predictive lifetime model for Fe-Al coatings on ferritic and austenitic alloys recognizing that a minimum acceptable coating lifetime for a commercial power plant is 40,000h (~5yr). The long-term scope of the coating work is to further develop and verify the lifetime prediction methodology for model coatings and then develop a similar predictive approach for low cost commercial scale coating processes (e.g. slurry coatings and pack cementation) while incorporating the potential influence of creep and fatigue on lifetime. The benefit of this lifetime model will be to more clearly define the potential benefits for Al-containing coatings to industry in terms of service time for a given set of environmental and coating conditions. For the alloy development work, one potential outcome is a new class of oxidation-resistant Fe-base alloys. However, a better fundamental understanding of the critical mechanisms may ultimately be more useful in incrementally improving the performance of current alloys and in developing better Al-containing coatings.

Keywords: Alloys, Coatings, Lifetime

272. HIGH-TEMPERATURE CORROSION RESISTANCE OF Fe-Al-Cr WELD OVERLAY COATINGS (LU-2)
$120,000
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The scope of this project deals with the protection of materials that will be used in the construction of both the waterwall and superheater components in advanced steam boilers. The two candidate materials of interest are ASTM 213 T-92 and T-23. As well as being implemented for the waterwall section, there is interested in extending the higher chromium T-92 alloy into the superheater section. This is of important concern. Compared to the sulfidzing environment of the waterwalls, alloys in the superheater regions will be exposed to higher temperatures in an oxidizing environment. The changes in environment alter the main mode of corrosion from sulfidation to coal-ash corrosion. This introduces a whole new corrosion mechanism for the Fe-Al-Cr overlays, and their corresponding behavior must be characterized. The scope of this project is divided into two main parts. First, it is necessary to determine the weldability of Fe-Al-Cr alloys on the alloy substrates that will be implemented in the sections of interest for the ultra supercritical boilers. From the determined weldability range, candidate alloys must be selected. Second, the candidate alloys must be exposed to the low-NO_X conditions that will be seen in actual service. For alloys on the T-23 tubes this entails only exposure to the simulated waterwall environments. With the T-92 tubes, samples must be exposed to the sulfidizing environment of the waterwall area and the coal ash condition seen in the superheater areas. The corrosion behavior of all tested alloys will be characterized and for the superheater section compared to the typical alloys presently used in current boilers.

Keywords: Boilers, USC, Joining, Coatings, Oxidation

273. CHEMICALLY VAPOR DEPOSITED YSZ FOR THERMAL AND ENVIRONMENTAL BARRIER COATINGS (ORNL-1A)
$225,000

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Yttria-stabilized zirconia (YSZ) is critical for several technological applications. A 6 to 8 wt % Y_2O_3 (6.5 to 8.5 mol % $YO_{1.5}$) stabilized tetragonal-phase zirconia is used as a thermal barrier coating (TBC) on turbine blades for increasing the lifetime and efficiency of gas turbine engines. Currently, air plasma spray (APS) and electron-beam physical vapor deposition (EB-PVD) are the only two commercial methods for fabricating YSZ TBCs. APS appears to produce coatings with less mechanical stability and premature delamination. The EB-PVD technique produces longer lasting and more effective coatings, but this method requires significant capital investment and in general is more costly. Further, both coating methods have difficulty with low throughput capacity and in coating complex geometries, as they are line-of sight processes. In this work, a potentially more commercially viable technique, chemical vapor deposition (CVD), is investigated as an alternative to these processes. Metal-organic CVD (MOCVD) has been identified as a potentially more efficient process than either APS or EB-PVD, and is perhaps able to yield improved performance. Work at the University of Colorado, Canterbury University, and the Technical University of Braunschweig has demonstrated the feasibility of the approach.

Project performance indicators have been used at various project stages. Success of a project indicator was used as a key decision point to move on to the next stage. To date these have included using chemical thermodynamic modeling and the support of kinetics-fluid dynamics coupled reactor modeling to demonstrate that YSZ coatings could be successfully deposited. The follow-on indicator/decision point was the demonstration on small substrates (2-cm) of deposition of tetragonal-YSZ using chloride, and then metal-organic precursor systems. Thick coatings with columnar microstructures were then prepared, as these are necessary for adequate thermal protection and strain tolerance. Coatings with the appropriate microstructure were deposited on small substrates of candidate advanced turbine alloys (FeCrAlY) and tested in thermal cycling for up to 1000 cycles. Following the demonstrated success of both the desired coatings production and their 1000 cycle-plus lifetime, initial efforts to scale the process to coat prototypical scale blade cross sections of 12 cm have also been successful. Informed by the coupled kinetics-fluid dynamics modeling, a scale-up coating system was designed and constructed. Current efforts are to deposit uniform coatings with appropriate thickness and microstructure on the 12-cm substrates. Additional work will focus on coating specimens provided by Pratt & Whitney for burner rig testing. In parallel efforts, success with both scale-up will be accompanied by technology transfer to interested commercial firms, signifying successful termination of the project.

Keywords: YSZ, MOCVD, Coatings

274. MODELING OF CHEMICAL VAPOR-DEPOSITED ZIRCONIA FOR THERMAL BARRIER AND ENVIRONMENTAL BARRIER COATINGS (UOL-3)
$65,000

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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 alk-oxide 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 ORNL. 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, CVD

275. ALUMINIDE COATINGS FOR POWER-GENERATION APPLICATIONS (TTU-2)
$70,000
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The objectives of the project are to develop a comprehensive coating lifetime evaluation approach, and to improve long-term coating durability for coatings applicable to critical components in power generation processes. The approach being used is to investigate the critical issues associated with aluminide coatings on two major industrially-relevant alloy systems: Fe-based alloys, and Ni-based superalloys. For the Fe-based alloys, the long-term interdiffusion behavior between the coating and steel substrates (ferritic and austenitic) is being assessed to explore potential benefits of iron aluminide coatings in terms of lifetime and applicable environments. For the Ni-based superalloys, effort is focused on modifications to aluminide coatings to minimize interdiffusion with the superalloy during prolonged service at high temperatures. Pt-enriched $\gamma+\gamma'$ two-phase aluminides have been shown to have significantly different diffusion properties than the more commonly-used or γ'- or b-aluminides, but the compositional changes required are in the direction expected to compromise the ability to form the desired protective oxide scales. In addition to interdiffusion measurements and modeling, the coatings are being evaluated in laboratory corrosion tests to quantify their cyclic oxidation performance.

Keywords: Superalloys, Coatings, Pt-Enriched

276. INFLUENCE OF PROCESSING ON COATING MICROSTRUCTURE AND PROPERTIES (INEL-2)
$170,000
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The prime objective of this project is to develop improved fundamental understanding of the influences of thermal-spray coating materials and processing parameters on durability measures such as adhesion and cracking resistance. Although the potentially strong role of environment on durability is recognized, the focus is on mechanical aspects of coating durability rather than corrosion *per se*. The coating materials of interest have already been shown to possess excellent intrinsic corrosion resistance, and their lives will more likely be limited by mechanical factors. These materials include iron aluminide intermetallics and nickel-chromium coatings applied by high-velocity oxy-fuel spraying, and advanced Mo-Si-B alloys applied by plasma spraying.

Keywords: Intermetallics, Coatings, Plasma Spraying

277. CORROSION RESISTANT CERAMIC COATINGS (ORNL-1B)
$200,000
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Enhancing output and economics of fossil energy conversion and combustion system's, i.e., gasifiers, by operating at higher temperatures, higher throughputs, and variable feed stocks, decreases the useful operating life of the materials used in these environments. The limit of most "high temperature materials", i.e., ceramics, is the 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 mullite coatings on sintered alpha silicon carbide substrates and the Albany Research Center- developed chromia system on chromia refractory bricks.

Keywords: Ceramics, Coatings

278. DEVELOPMENT OF NONDESTRUCTIVE EVALUATION METHODS FOR CERAMIC COATINGS (ANL-1)
$215,000
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The goal of this project is to develop nondestructive evaluation (NDE) technologies 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-fired turbines. Of primary interest are thermal barrier coatings (TBCs) composed of yttria-stabilized zirconia (YSZ) for application to superalloy vanes, blades, and combustor liners. Such coatings are considered to be critical to the higher gas-firing-temperature turbines suggested for the DOE/Fossil Energy/FutureGen program. NDE technologies will be necessary to avoid shut-downs and unscheduled outages caused by TBC failures. A significant effort by many investigators has been placed on developing NDE technologies, and a majority of the development work to-date has focused on characterization of coatings produced using electron-beam physical vapor deposition (EB-PVD). However, for land-based, coal-gas fired power turbines, there is a higher interest in TBCs applied by air plasma spraying (APS). The reason is the size of the individual components and coating costs. One NDE technology that has received considerable attention for EB-PVD coatings is luminescence spectroscopy. Extensive scattering of the light within an APS coating tends to preclude application of this technology. Recent NDE work for APS coatings has investigated the use of dopants together with mid-infrared thermal imaging technology. The results were marginally successful. Use of dopants however has the side issue of establishing the effect the dopants have on the performance of the TBC. Establishing the concentration levels of dopants necessary as well as the effect on TBC performance remain as unanswered questions.

Keywords: Non-Destructive Evaluation, YSZ, Thermal Barrier Coating, Ceramics

FUNCTIONAL MATERIALS

279. LOW-CHROME/CHROME FREE REFRACTORIES FOR SLAGGING GASIFIERS (ARC-1)
$200,000
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Past program research has focused on determining critical issues in the wear of gasification refractories, the role chrome oxide plays in current hot face linings, and on selecting and evaluating potential non-chrome oxide liner materials for use as improved or alternative liner materials. There are several continuing issues with Cr_2O_3 refractory materials used in air-cooled slagging gasifiers, which include: a) current high-Cr_2O_3 containing refractories do not meet the performance requirements of gasifier users, b) perceived/real long term safety concerns associated with the use of Cr_2O_3 refractory materials and their interaction with slags, c) the high cost associated with refractory materials containing high-Cr_2O_3 content, and d) possible long-term domestic supply issues. To address these and other concerns, this research project is investigating and developing low-chrome/no-chrome oxide liner materials for use in slagging gasifiers. These goals will be achieved by: 1) investigating the role chrome oxide plays in gasifier refractories, 2) evaluating wear mechanisms that play a role in gasifier failure, 3) evaluating non-chrome or low-chrome high temperature refractory oxides with potential for use in combating known wear mechanisms in gasifier refractories, 4) developing and evaluating engineered refractory shapes containing low or no chrome oxide, and 5) conducting field tests of these engineered refractory materials.

Keywords: Refractories, Gasifiers, Chrome

280. DEVELOPMENT OF NOVEL ACTIVATED CARBON COMPOSITES (ORNL-3E)
$330,000
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With increasing emphasis being placed on the development of fuel cells, coal-derived synthesis gas is a potential major source of H_2. Oxygen-blown coal gasification is the most effective and efficient approach to achieving the goal of producing H_2 from coal, but a more cost-effective means of enriching O_2 concentration in air is required. A key objective of this project is to assess the utility of system that exploits a porous carbon material and electrical swing adsorption (ESA) to produce an O_2-enriched air stream suitable for coal gasification. Technical performance indicators include development of an adsorbent with pronounced molecular sieving properties to obtain effective separation of O_2 and N_2 from air, and with the desired electrical characteristics to exploit the ESA technique to obtain a seamless production of an O_2-enriched air stream.

Keywords: Carbon, ESA, Coal Gasification, Molecular Sieve

281. DEVELOPMENT OF INORGANIC MEMBRANES FOR HYDROGEN SEPARATION (ORNL-3B)
$245,000
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The purpose of this work is to improve the method of fabricating tubular metal supported microporous inorganic membranes. Earlier work focused on the original development of these membranes which are now being scaled up for demonstration in a coal gasification plant for the separation of hydrogen from coal-derived synthesis gas for a project funded by the Office of Fossil Energy's Gasification and Coal Fuels programs. This project is part of FutureGen, an initiative to build the world's first integrated sequestration and hydrogen production research power plant. Although previous work in the Advanced Research Materials Program project lead to development of a tubular metal supported microporous membrane based on ORNL technology which was approved by the Department of Energy for testing, the membranes generally have lower than desired selectivities for hydrogen over other gases including carbon dioxide. The work on this project over the next three years will lead to general improvements in fabrication techniques that will lead to membranes having higher separation factors and higher fluxes.

Keywords: Membranes, Hydrogen Separation

282. THE PRODUCTION OF PURE HYDROGEN FROM HYDROCARBONS (LANL-3)
$100,000
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Hydrogen-separating membranes have the potential to facilitate the generation of pure hydrogen for use in fuel cells. LANL is collaborating with Ames Laboratory to develop porous membranes made from iron aluminide microparticles. The membrane will serve as a support for a palladium film that is thinner and more thermally tolerant. Collaboration on membranes based on Group V metals such as vanadium includes REB Research & Consulting (www.rebresearch.com). Synergistic collaboration enables the project to benefit from a multidisciplinary viewpoint and collective membranes experience. Recent important results regarding the long-term hydrogen permeability of a palladium coated V-6Ni-5Co membrane have shown that, at 400˚C, the flux was essentially constant for more than 500 hrs. This increased stability is a significant improvement over Pd-coated pure vanadium membranes. A value of $1.5E^{-4}$ mol m^{-2} s^{-1} $Pa^{-0.5}$ for hydrogen permeance was obtained. For the hydrogen flux test at 450˚C, the hydrogen flux was fairly constant with no apparent flux decrease for about 100 hrs, followed by a slow, steady decrease over the next ~500 hrs of testing. The membrane tested at 500˚C was first tested over a period of 64 hrs at 400˚C, and then the temperature was increased to 500˚C. During only 41 hrs of exposure to hydrogen at 500˚C, the flux decreased rapidly to less than half its highest value, 0.054 mol m^{-2} s^{-1}, measured at 400˚C. The flux decreased more quickly than at 450˚C, presumably due to an increase in the rate of metallic interdiffusion. RBS and AES depth profile analysis were both very helpful for studying the metallic interdiffusion between the V foil and the Pd coating. These studies are providing important insight into the mechanisms of metallic interdiffusion.

Keywords: Alloys, Membranes, Hydrogen Separation

283. GAS SENSORS FOR FOSSIL ENERGY APPLICATIONS (ORNL-3H)
$235,000
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The objective of this project is to develop a low-cost electrochemical sensor based on mixed potential phenomena that will detect SO_2, SO_3 and/or total SO_x at temperatures from 500-600˚C. The research will follow a logical progression from: the catalytic evaluation of mixed conducting oxide powders; the evaluation of the kinetics at the surfaces of these materials under the influence of applied electric potentials; the development of sensors based on the materials, and finally, testing of the sensors developed. Measurement of sulfur dioxide is a serious global problem in relation to environment pollution, occupational and public heath, and industrial emissions control. SO_2 is a major atmospheric pollutant resulting from the combustion of fossil fuels. It produces acidity in rainwater and is a major source of corrosion in buildings. The major health concerns associated with exposure to high concentrations of SO_2 are respiratory illness, alteration of the lungs defenses, and aggravation of existing cardiovascular disease. One of the first steps towards solving these environmental and health problems is measuring the concentration of these gases in many locations. Thus, there is an increasing interest in the development of simple, inexpensive and reliable methods for the analysis and monitoring of SO_2. Gas sensors are needed to control advanced combustion and gasification systems and for environmental controls of power plans. Other key sensors include NO_x, ammonia and mercury.

Keywords: Sensors, Gasification

284. SEALING TECHNOLOGY FOR GAS SEPARATION MEMBRANES (PNL-3)
$350,000
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The primary objective of this project is to develop the joining/sealing technology required for high-efficiency, low-emissions fossil energy conversion, in support of the Department of Energy-Office of Fossil Energy's (DOE-FE) Clean Coal Utilization and FutureGen programs. This project is focused on developing the seals needed to hermetically join the various inorganic membranes and support structures that are currently being considered for use in high-temperature gas separation systems. Membrane materials under development include microporous alumina and mixed ionic/electronic conducting oxides (MIECs) for the separation of hydrogen from coal gas and syngas, and perovskite and brownmillerite MIECs for the separation of oxygen from air. The sealing materials chosen for use in a high-temperature gas separation device must be capable of withstanding the transient and steady-state operating conditions (including a nominal temperature of 700˚C), exposure to oxidizing (oxygen separation) and/or reducing (hydrogen extraction) conditions, and numerous thermal cycles, and achieve a lifetime of tens of thousands of hours. There are two current routes for such joining: 1) glass bonding, for which the maximum operating temperature is limited by the softening point of the glass. At present, high-temperature glasses with appropriately matching coefficients of thermal expansion are limited to a narrow range of compositions within the borate-doped aluminosilicate family, and these typically display signs of devitrification within the first few hours of exposure at operating temperature; and 2) active metal brazing, which uses a filler metal that, when heated above its liquidus temperature, will flow and fill the gap between the two joining pieces by capillary action. Unlike metal-to-metal brazes, this family of braze alloys contains one or more reactive metals (often Ti) which will chemically reduce the ceramic at the interface with the braze, greatly improving wetting and adherence between the two materials. However, there are significant problems with using active metal brazing for the fabrication of solid-state electrochemical devices: i) the complete oxidation of the active species in the braze during high-temperature operation of the device will lead to rapid deterioration of the joint at the ceramic/braze metal interface and an eventual loss in hermeticity; ii) exposure of the entire device to a reducing atmosphere at a temperature greater than ~800˚C (typical processing conditions for active metal brazing) has been found to be too demanding for many of the oxide materials employed in these devices; iii) some oxides will tend to reduce during the joining operation, which can cause irreversible deterioration of the functional ceramic. To overcome these difficulties, an alternative method of ceramic-to-metal brazing ("air brazing") is being developed. This technique differs from traditional active metal brazing in two important ways: (a) it utilizes a liquid-phase oxide-noble metal melt as the basis for joining and, therefore, exhibits high-temperature oxidation resistance, and (b) the process is conducted directly in air without the use of fluxes and/or inert cover gases. The technique employs a molten oxide (that is at least partially soluble in a noble metal solvent) to pre-wet the oxide faying surfaces, forming a new surface that the remaining molten filler material easily wets. Development is progressing along two distinct paths: (1) studies to explore how the base Ag-CuO filler metal can be modified to alter the metallurgical and brazing properties (such as lqiuidus/solidus temperature, wettability, joint strength, and maximum exposure temperature of the joint), and (2) investigation of air-brazed joint properties, specifically hermeticity as a function of coal gas exposure. The general approach over the past year has been to focus primarily on membranes for hydrogen separation, in particular, microporous alumina.

Keywords: Membranes, Gas Separation, Brazing

BREAKTHROUGH CONCEPTS

285. MULTI-PHASE, HIGH-TEMPERATURE ALLOYS: EXPLORATION OF LAVES-PHASE STRENGTHENED STEELS (ORNL-2D)
$110,000
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The overall objective of this effort is to develop high-strength, oxidation- and corrosion-resistant alloys for use in advanced fossil energy conversion and combustion systems to permit higher operating temperatures to help meet efficiency increase and emission reduction goals. The alloy design strategy is based on the manipulation and control of multi-phase structures, and the concurrent development of improved mechanical properties, particularly creep strength, and oxidation/corrosion resistance. The current effort is to develop intermetallic Laves phase-strengthened austenitic alloys for improved elevated-temperature creep strength. Advanced fossil energy power plants call for austenitic stainless steels capable of operation at temperatures greater than 700˚C. A key challenge is the concurrent development of creep strength and oxidation resistance, especially in oxidizing environments also involving exposure to sulfidation, hot corrosion, or water-vapor species. Alumina-based scales are of particular interest due to their superior resistance to water vapor-containing environments, compared to chromia-based scales, which are susceptible to accelerated oxidation due to volatilization-related effects. Al-modified austenitic alloys have been explored intermittently in the past. However, it has proven difficult to achieve creep strengthening due to the strong BCC stabilizing effects of Al, and concomitant potential for ferrite formation, interference with interstitial nitrogen additions used to enhance strengthening in austenitic alloys (by the formation of AlN), and a tendency to increase stacking fault energy and cross-slip. Welding of previously developed Al-modified alloys has also proven difficult. Oxidation studies under the current effort were therefore directed toward assessment of scale formation with relatively low additions of Al (2-3 wt.%), in order to minimize the detrimental effects of Al on strengthening. Benchmarking and decision points are based on comparison with the type 347 family of stainless steel alloys (18Cr-10Ni wt.%), which is considered for baseline purposes, and the 20Cr-25Ni family such as NF709, which represents the current state of the art for creep- and oxidation- resistant austenitic stainless steel alloys.

Keywords: Alloys, High Temperature, Oxidation, Stainless Steel

286. Mo-Si-B ALLOY DEVELOPMENT (ORNL-2I)
$140,000
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Mo-Si-B silicides consisting of a-Mo (Mo solid solution), Mo_3Si, and Mo_5SiB_2 have significant potential as ultra-high temperature structural materials. They can be processed such that the a-Mo is present in the form of isolated particles in a silicide matrix, or as a continuous matrix "cementing" individual silicide particles together. The demands for good oxidation resistance on the one hand, and good fracture toughness on the other, are difficult to satisfy at the same time. If the ductility of the a-Mo phase can be improved, less a-Mo will be required to achieve a certain value of the fracture toughness, and therefore the oxidation resistance is expected to improve. Potential ductilization mechanisms include (a) alloying with zirconium and (b) incorporation of $MgAl_2O_4$ spinel particles. Mo-2.5 at% Si alloys with two different Zr concentrations were prepared by arc-melting. In spite of high silicon (which is expected to lead to embrittlement) they showed satisfactory room temperature fracture toughness values on the order of 20 MPa $m^{1/2}$. In the case of $MgAl_2O_4$ additions, the room temperature ductility of Mo-2.5 vol% $MgAl_2O_4$ was much higher than that of Mo-0.1 vol% $MgAl_2O_4$. This is the first independent verification of the ductility improvement of Mo by $MgAl_2O_4$ since it was first suggested by D. M. Scruggs in 1967. However, the ductility improvement may not be due to impurity gettering as proposed by Scruggs. Also, since the fracture mode in our experiments was intergranular, higher ductility values may be attainable. Further improvements in the balance of properties for Mo-Si-B alloys appear thus feasible.

Keywords: Alloys, Mo-Si-B, Corrosion

287. INFLUENCE OF IMPURITIES ON DUCTILITY OF Cr- AND Mo-BASED ALLOYS AND IN-SITU MECHANICAL PROPERTY MEASUREMENT (WVU-2)
$140,000
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Since even a tiny amount of impurities can cause dramatic changes in mechanical properties of high strength metallic alloys. Despite a long history of discovery, a large proportion of the fundamental mechanisms remains poorly understood. This places severe obstacles in designing and optimizing high strength structural alloys for fossil energy applications. This project consists of both theoretical and experimental research tasks with the aim to understand the fundamental mechanisms of nitrogen or oxygen embrittlement of Cr and Mo alloys and ductility enhancement by MgO dispersions, as recently demonstrated in experiments conducted by Brady, et. al. at ORNL. On the theoretical task, using computational atomistic modeling techniques, we aim to develop predictive capabilities to facilitate the design and optimization of high-temperature structural alloys for fossil energy applications. As for the experimental task, we have developed a transparent indenter measurement technique for quick assessment of material mechanical properties of alloys relevant to Advanced Research Materials Program, thus providing feedbacks for the design and further optimization of future material systems to meet the ever growing demands of fossil energy applications.

Keywords: Alloys, Chromium, Mechanical Properties, Modeling

288. NOVEL PROCESSING OF Mo-Si-B INTERMETALLICS FOR IMPROVED EFFICIENCY OF POWER SYSTEMS (AMES-2)
$75,000
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Bcc-Mo-based Mo-Si-B alloys have promising high-temperature mechanical properties. In particular, the bcc-Mo+T2(Mo_5SiB_2)-based alloys have excellent resistance to fracture, with toughness values approaching 20 MPa·$m^{½}$ for a continuous -Mo matrix material. However, a fundamental limitation of these alloys is their poor oxidation resistance at temperatures envisioned for critical applications in, for instance, coal gasification environments.

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, Coal Gasification

289. STUDY OF FATIGUE AND FRACTURE BEHAVIOR OF Ti-Al-Nb-W-B INTERMETALLIC MATERIALS (UT-2A)
$95,000
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The TiAl alloys have been considered as promising candidates for structural-materials applications at around 800˚C. In this work, new TiAl alloys, containing tungsten (W) and boron (B), have been developed. Using the scanning-electron microscopy, electron-microprobe, and transmission-electron microscopy, the effects of W and B on the microstructural evolution of TiAl alloys, including the colony size and lamellar spacing, were analyzed. It is important to point out that fine uniform microstructures (with the colony size smaller than 50 mm) can be conveniently developed after Hot-Isostatic Pressing the as-cast alloys at 1,250˚C and 150 MPa for 4 h without a deformation process. It was found that W prefers to react with B to form borides, and disperses mainly along grain boundaries, and occasionally inside grains. With increase of the W content, the microstructure can be further refined. Heat treatments at temperatures ranging from 900 to 1,310˚C were conducted. The addition of W can restrain grain coarsening and stabilize the microstructure up to 1,280˚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 W content exceeds 0.4 at.%. The α-phase transus temperature, T_α, has been determined through differential-thermal analyses and further proved by the 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 experiments, has been conducted on the alloys. The addition of the alloying element, W, increases the hardness of TiAl alloys by solution strengthening and refinement of grain size.

Keywords: Intermetallics, Alloys, Microstructure, Tungsten

290. NOVEL STRUCTURES AND PROPERTIES THROUGH CONTROLLED OXIDATION (ORNL-4A)
$200,000
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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.

Keywords: Oxidation, Alloys, Ceramic

291. CONCEPTS FOR SMART, PROTECTIVE, HIGH-TEMPERATURE COATINGS (ORNL-4C)
$120,000
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The purpose of this work is to assess the feasibility of different material and design approaches to smart protective coatings by exploring new alloying and microstructural routes to improved high-temperature environmental resistance of metallic materials. As such, this work supports the overarching goal of the Fossil

Energy Advanced Research (AR) Materials Program to provide a materials technology base to assure the success of coal fuels and advanced power generation systems being pursued by the Office of Fossil Energy. This specific project is motivated by need for materials with improved high-temperature environmental resistance that could be used as protective coatings under the harsh conditions encountered in advanced fossil systems. Historically, the development of materials for fossil-fuel combustion and conversion systems has been closely linked to corrosion studies of alloys and ceramics in appropriate environments so as to identify reaction or degradation mechanisms and develop and/or select materials that offer improved performance. This task, however, differs in that it evaluates the feasibility of new routes to controlling the critical chemical and mechanical phenomena that collectively form the basis for corrosion resistance in relevant fossil environments by exploring compositional and microstructural manipulations and cooperative phenomena that have not necessarily been examined in any detail to date. Its goal is not to develop coatings per se. Rather, it is to examine concepts that can then be translated into coatings by further developmental efforts if promising high-temperature corrosion results are found for a particular composition/microstructure combination (and possible synthesis routes can be identified). As such, this work is positioned at the breakthrough/high risk/far-term end of the spectrum that represents the intended scope of the AR Materials program. The first concepts 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 showed generally good oxidation and sulfidation resistance.

Keywords: Coatings, Alloys, Oxidation, High Temperature

292. PILOT FACILITY FOR THE PRODUCTION OF SILICON CARBIDE FIBRILS (REMAXCO-5)
$100,000
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Single crystal silicon carbide fibrils have exhibited oxidation resistance to 1,600˚C 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-fire combustion plants. A manufacturing process for these fibrils with the potential for low cost and high volume fibril production is being investigated. Two previous fibril growth equipment designs have shown that the microwave process grows the fibrils at three times the rate of the previous process, with a minimal use of raw materials and energy. The process has been demonstrated to work. The 3rd-generation reactor is an improved design of the previous two and was built to test the efficiency of the process. Raw material consumption and energy use will be measured as a function of volume of fibrils produced to determine the actual projected unit cost of volume production. Key decision points will be based on the unit cost factors, namely: whether the equipment or processing parameters be improved to lower cost, and the potential to scale-up the process to ton quantities per year at reasonable capital equipment costs. If these changes offer a high probability of success, funds will be spent on improving the 3rd generation reactor or building a 4th generation reactor. If scaling to volume production is cost prohibitive or if the volume unit cost is shown to be above $500/pound, the project will be terminated at the conclusion of the testing of the current reactor performance.

Keywords: SiC, Fibrils, Composites

293. ADVANCED PROCESSING OF METALLIC POWDERS (AMES-3)
$70,000
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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, 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) powders 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 an advanced industrial operation in terms of steady state operation and controls 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-base 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, Membranes, Powders

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.

Keywords:

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

294. 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

295. EFFECT OF REACTIVE ELEMENT SURFACE INFUSION ON THE OXIDATION BEHAVIOR OF ALLOYS
$200,000
DOE Contact: Alan D. Hartman, (541) 967-5862
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Research investigates several aspects relating to issues associated with the infusion technique and fundamental aspects relating to the effect of reactive elements on oxidation behavior. Research will be conducted to determine influence of alloy chemistry and structure on the oxidation behavior of the infusion method. Research will also be conducted to evaluate the ARC infusion method on the behavior of commercial alloys relevant to fossil energy applications. The final element will systematically determine the fundamental reason for the improvement in resistance of alloys with rare earth alloying additions.

Keywords: Alloys, Castings, Rare Earth Elements

296. HIGH TEMPERATURE STRENGTHENING CONCEPTS IN HIGH PERFORMANCE MATERIALS FOR ENERGY APPLICATIONS
$315,000
DOE Contact: Alan D. Hartman, (541) 967-5862
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In order to achieve increased efficiency in all forms of energy generation, systems must operate at higher temperatures and pressures. The overarching limitation to achieving this goal is a lack of adequate metallic materials that can withstand these temperatures and pressures. As such, research will be conducted utilizing thermodynamic and kinetic modeling coupled with conventional melting and casting practice to produce ferritic/martensitic steel, austenitic steel, nickel alloys and other high temperature metallic materials. These materials are envisioned to be used for extending the operating envelop of existing power generating components, including fuel cells, sub-critical, super-critical and ultra-super critical power plants.

Keywords: Alloys, Castings, Steel, Nickel

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
$500,000
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
$1,000,000
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
$1,000,000
DOE Contact: Alan D. Hartman, (541) 967-5862
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The chief characteristic of fuel cells is the ability to convert chemical energy to electrical energy without the need for combustion, giving much higher conversion efficiencies than conventional methods. Costs of fuel cells remain an issue and can be reduced in component fabrication, materials used, and cell and stack designs. 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

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