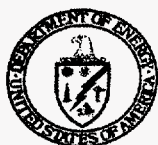
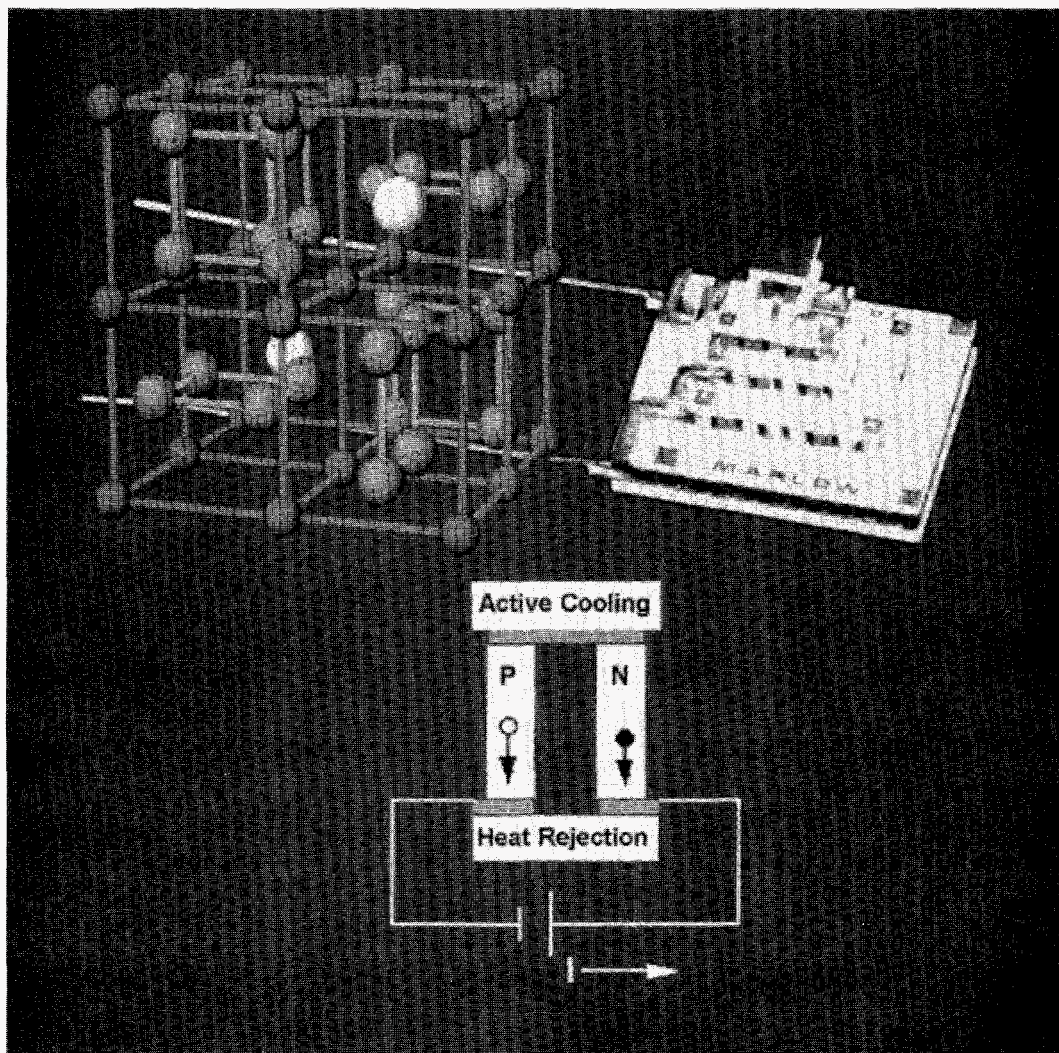


---

## LABORATORY TECHNOLOGY RESEARCH

### Abstracts of FY 1998 Projects

---



U. S. Department of Energy  
Office of Science  
Office of Computational and Technology Research  
Advanced Energy Projects and Technology Research Division  
Germantown, MD 20874-1290

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

### **DISCLAIMER**

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

## **DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

## TABLE OF CONTENTS

### LABORATORY TECHNOLOGY RESEARCH PROGRAM

|   |     |
|---|-----|
| Program Overview .....                                  | iii |
| Program Focus Areas .....                               | iv  |
| Advanced Materials .....                                | iv  |
| Intelligent Processing and Manufacturing Research ..... | iv  |
| Environmental and Biomedical Research .....             | v   |
| Major Industry Partnerships .....                       | vi  |

### PROGRAM IMPLEMENTATION

|                                   |     |
|-----------------------------------|-----|
| Multi-Year Projects .....         | vii |
| Rapid Access Projects .....       | vii |
| Major Industry Partnerships ..... | vii |

### CONTACTS FOR THE LTR PROGRAM

|                                      |      |
|--------------------------------------|------|
| U.S. Department of Energy .....      | viii |
| Office of Science Laboratories ..... | viii |

### ABSTRACTS OF MULTI-YEAR PROJECTS SUPPORTED IN FY 1998

|  |    |
|--|----|
| Advanced Materials   |    |
| Design of Materials .....                                  | 1  |
| Advanced Synthesis and Characterization Technologies ..... | 9  |
| Films and Coatings .....                                   | 13 |
| Energy Conversion and Storage .....                        | 22 |
| Intelligent Processing and Manufacturing Research          |    |
| Intelligent Design .....                                   | 32 |
| Intelligent Manufacturing Processes .....                  | 34 |
| Enabling Technologies .....                                | 41 |
| Environmental and Biomedical Research                      |    |
| Biotechnology .....  | 50 |
| Medical Technologies .....                                 | 52 |
| Cleaner Industrial Processes .....                         | 62 |
| Environmental Technologies .....                           | 76 |
| Major Industry Partnerships                                |    |
| Advanced Computational Technology Initiative (ACTI) .....  | 79 |
| American Textiles (AMTEX) Partnership .....                | 85 |

### EXAMPLES OF RAPID ACCESS PROJECTS

|                            |    |
|----------------------------|----|
| Personnel Exchange .....   | 92 |
| Technical Assistance ..... | 93 |
| Small CRADAs .....         | 95 |



|  |     |
|--|-----|
| APPENDIX A - CROSS REFERENCE TABLE FOR MULTI-YEAR PROJECTS ..... | 97  |
| APPENDIX B - ALPHABETICAL LIST OF INDUSTRIAL PARTNERS .....      | 98  |
| APPENDIX C - ALPHABETICAL LIST OF PRINCIPAL INVESTIGATORS .....  | 101 |

# LABORATORY TECHNOLOGY RESEARCH PROGRAM

## Program Overview

The Laboratory Technology Research (LTR) program supports high-risk, multidisciplinary research partnerships to investigate challenging scientific problems whose solutions have promising commercial potential. These partnerships capitalize on two great strengths of our country: the world-class basic research capability of the DOE Office of Science (SC) national laboratories and the unparalleled entrepreneurial spirit of American industry.

A distinguishing feature of the SC laboratories is their ability to integrate broad areas of science and engineering in support of national research and development goals. The LTR program leverages this strength for the Nation's benefit by fostering partnerships with U.S. industry. The partners jointly bring technology research to a point where industry or the Department's technology development programs can pursue final development and commercialization.

Collaborative research projects supported by the LTR program are partnerships: the program funds only the national laboratory's research, while the industrial partner supports its research and often provides equipment, funds, or supplies to the laboratory. Thus, a laboratory and its industrial partners can explore scientific and technical approaches that would be too risky for industry to undertake alone. Such work leverages the resources of both partners, since each frequently has unique and complementary facilities and expertise. The LTR program enhances opportunities to pursue technology research that is of value to industry, complements basic research program goals, and seeks to enhance public benefit from investment in scientific research at the national laboratories.



The LTR Program has won  
20 R&D-100 Awards

The scientific impact of the LTR program has already been dramatic. Since its inception in 1992, the program's technologies have won 20 R&D-100 Awards, 15 Federal Laboratory Consortium Awards, and eight other awards, such as those from Popular Science and Discover magazines. The record of R&D-100 Awards exemplifies the steadily increasing success of these cooperatively developed technologies.

Projects supported by the LTR program in FY 1998 were conducted by the five major SC multi-program laboratories: Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge, and Pacific Northwest National Laboratories.<sup>+</sup> These projects explore the applications of basic research advances relevant to DOE's mission over a full range of scientific disciplines. The program presently emphasizes three critical areas of mission-related research: advanced materials, intelligent processing and manufacturing research, and environmental and biomedical research.

---

<sup>+</sup>At the beginning of FY 1999, the following five laboratories were reinstated into the LTR program: Ames Laboratory, Fermi National Accelerator Laboratory, Princeton Plasma Physics Laboratory, Stanford Linear Accelerator Center, and Thomas Jefferson National Accelerator Facility.

## **Program Focus Areas**

### **Advanced Materials**

The Advanced Materials portion of the LTR program will provide a strong foundation for advances in many areas of science and technology including energy, transportation, manufacturing, health, and the environment. Using synthesis, processing, and characterization techniques and advanced computational tools for design and modeling coupled with the integration of basic and applied disciplines, this research will result in the improvement of existing materials and the development of new materials and knowledge of their properties. Research focuses on a broad range of materials problems related to ceramics and composites, metals and alloys, surfaces and thin films, nanomaterials, polymers and biomaterials, and superconducting materials. Results support DOE missions in basic science, energy efficiency, fossil energy, fusion energy, environmental management, and national security. The research is intended to complement, enhance, and leverage existing DOE materials programs through research partnerships.

Advanced materials research focuses on four major subtopics.

- **Design of Materials:** Emphasis is placed on modeling and characterization; alloying and doping; composite and functional graded materials; and nanostructures. This includes materials that respond to external stimuli, such as shape memory alloys, and magneto-resistant, piezoelectric, and electro-rheologic materials.
- **Advanced Synthesis and Characterization Technologies:** Emphasis is placed on advanced techniques such as ion, plasma, laser, and MBE techniques and environmentally friendly processing techniques that reduce waste and/or energy consumption.
- **Films and Coatings:** Emphasis is placed on surface modification, corrosion and wear resistance, and multilayered films.
- **Energy Conversion and Storage:** Emphasis is placed on materials that can be used for the manufacture and processing of fuels, as well as the development of materials useful in the construction and improved performance of batteries and fuel cells.

### **Intelligent Processing and Manufacturing Research**

Intelligent Processing and Manufacturing Research (IPMR) is a multidisciplinary activity which integrates and builds upon the results of DOE basic research to develop new and advanced processing and manufacturing technologies required to meet DOE missions.

The goal of IPMR is to perform technology research projects that apply core DOE laboratory capabilities to advance the state of intelligent processing and manufacturing. To meet this goal, research is conducted on a range of technology areas that include advanced sensors and controllers, computational technologies, and algorithms coupled with manufacturing processes. Research projects typically have applications in multiple manufacturing sectors and support DOE missions in science and technology, as well as energy and environment. IPMR projects also benefit national initiatives related to manufacturing such as Technologies Enabling Agile Manufacturing (TEAM), Next Generation Manufacturing (NGM), and the Partnership for a New Generation of Vehicles (PNGV).

IPMR focuses on four major subtopics.

- **Intelligent Design:** Emphasis is placed on modeling and simulation and on rapid prototyping.
- **Intelligent Manufacturing Processes:** Emphasis is placed on joining, forming, forging, and casting; and microfabrication.
- **Enabling Technologies:** Emphasis is placed on intelligent measurements, intelligent controls, and agile automation.

### **Environmental and Biomedical Research**

A new generation of environmental and biomedical technologies is needed that will enhance the general population's quality of life. This research area combines environmental technologies such as: pollution prevention, efficient resource use, and industrial ecology as well as biomedical technologies including radiopharmaceuticals and biomaterials. Such technologies can help companies become more competitive by lowering resource and energy needs, reducing waste and emissions control costs, and fostering sustainable development while enhancing the general health and well being of the general populace. SC supported programs in biotechnology, chemical and materials sciences, and novel energy concepts provide a fertile ground for further investigation for potential commercial application. Priorities for research in this area stress technologies that emphasize sustainable use of natural resources and avoidance of environmental harm as well as more effective biomaterials and medical technologies. These may include technologies to control and minimize environmental harm (particularly hazardous wastes), biomaterials with improved performance, efficacious radiopharmaceutical delivery systems, as well as environmental monitoring and remediation technologies.

Research on environmental and biomedical research focuses on four major subtopics.

- **Biotechnology:** Emphasis is on furthering developments in understanding the microbial and biochemical mechanisms that can contribute to solving complex bioprocessing problems. Topics in molecular biology, biochemistry, and microbiology fall into this category. A potential area for

investigation may be the application of extremophile bacteria to the degradation of toxic wastes.

- **Medical Technologies:** Emphasis is placed on health related technologies. Topics in this area include diagnostic technologies, biomaterials, and biomedicine. A potential area for investigation would be novel radiopharmaceuticals or superior materials for use as artificial bones.
- **Cleaner Industrial Processes:** Emphasis is placed on both experimental and computational capabilities in the development of environmentally benign industrial processes. This topic may span a variety of technologies from the application of modeling tools in the development, at the structural level, of new classes of catalysts, to large scale industrial process modeling.
- **Environmental Technologies:** Emphasis is on analytical methods, as well as processes and materials technologies with the goal to characterize and remediate polluted areas.

### **Major Industry Partnerships**

These partnerships team scientists and engineers in DOE national laboratories with an industry sector to research generic problems facing that industry. This is divided into two areas: the American Textiles (AMTEX) Partnership and the Advanced Computational Technology Initiative (ACTI) Partnership.

- **AMTEX Partnership:** The mission of AMTEX is to infuse technology into the integrated textile and apparel industry to offset foreign competition from low labor rates. Examples of these technologies are on-line inspection of cloth as it comes off the loom, using the Internet to connect buyers and sellers, and providing removable protective coatings for fibers to allow them to survive the weaving process.
- **ACTI Partnership:** ACTI pursues advanced computational technology for finding, developing, and producing natural gas and oil. This technology is directed towards the discovery and recovery of oil and gas by supporting borehole seismic, oil recovery, and drilling with the goal of enhanced production of natural gas and oil.

## PROGRAM IMPLEMENTATION

The LTR program conducts research using three different mechanisms:

- **Multi-Year Projects.** These cost-shared projects between SC laboratories and private industry are performed in support of DOE missions but also are relevant to industry needs. LTR program funding to SC laboratories for these projects is typically from \$100,000 to \$250,000 per year for a three-year period. The industrial partner supports its research in at least an equivalent amount. Cooperative Research and Development Agreements (CRADAs) are used to implement these projects. CRADAs provide for protection of proprietary data and disposition of intellectual property. Projects that were initiated in Fiscal Year (FY) 1998 were chosen by an external peer review of proposals on the basis of scientific/technical merit and commercial potential. The reviewers were practicing experts in the subject area of the proposal, from at least three different institutions, who did not have a conflict of interest. Each reviewer provided comments on four evaluation criteria: scientific/technical quality, qualifications of key personnel and facilities, the work plan, and commercial potential. A fifth criterion on the industry partner commitment to the project (either funds-in or in-kind support) was evaluated by the DOE LTR program based on commitment letters from the industry partner. Proposals which received the strongest evaluations overall were chosen for funding.

All of the multi-year projects which received FY 1998 funding from the LTR program (Total = \$10.5 million) are included in this book of abstracts. The following ID codes for each abstract identify the national laboratory conducting the project: ANL - Argonne National Laboratory, BNL - Brookhaven National Laboratory, LBL - Lawrence Berkeley National Laboratory, ORL - Oak Ridge National Laboratory, and PNL - Pacific Northwest National Laboratory.

- **Rapid Access Projects.** These projects provide private industry, especially small businesses, with a means to solve difficult technical problems rapidly by tapping the unique expertise of SC laboratory scientists and engineers. These projects are implemented through a variety of flexible mechanisms, such as personnel exchanges, technical assistance to and consultations with small businesses, and small collaborative projects (CRADAs). Funding is allocated on the basis of a merit review that emphasizes scientific/technical quality, commercial potential, and contribution to DOE's missions. These projects last from a few days to one year with LTR program funding to SC laboratories from \$3,000 to \$100,000 per project. Selected examples of each type of rapid access project are included in this book of abstracts. The total funding for rapid access projects was \$1.3 million in FY 1998.
- **Major Industry Partnerships.** Major industry partnership projects funded by the LTR program (Total = \$1.9 million) are part of a large group of projects focused on one industrial segment. Abstracts of multi-year projects in support of the ACTI Partnership, which received FY 1998 funding from the LTR program, are listed as project numbers 70 - 74. Abstracts of multi-year projects in support of the AMTEX Partnership, which received FY 1998 funding from the LTR program, are listed as project numbers 75-80.



## CONTACTS FOR THE LTR PROGRAM

### **U.S. Department of Energy**

Dr. Walter M. Polansky, Director

Advanced Energy Projects and Technology Research Division

Office of Computational and Technology Research

Dr. Samuel J. Barish, Team Leader

Laboratory Technology Research Program

Dr. Theodore Vojnovich

Dr. Dan Melamed<sup>♦</sup>

Ms. Bernadette Crehan

Advanced Energy Projects and Technology Research Division

U.S. Department of Energy, SC-32

19901 Germantown Road

Germantown, MD 20874-1290

Phone: (301) 903-7485

Fax: (301) 903-6067 (no more than 10 pages)

E-mail: walt.polansky@oer.doe.gov

sam.barish@oer.doe.gov

ted.vojnovich@oer.doe.gov

dan.melamed@oer.doe.gov

bernadette.crehan@oer.doe.gov

### **Office of Science Laboratories<sup>+</sup>**

#### **Ames Laboratory**

Mr. Robert S. Harris, Manager

SC LTR Program

Ames Laboratory

Iowa State University

311 TASF

Ames, IA 50011

---

<sup>♦</sup>On detail from Brookhaven National Laboratory

<sup>+</sup>At the beginning of FY 1999, the following five laboratories were reinstated into the LTR program: Ames Laboratory, Fermi National Accelerator Laboratory, Princeton Plasma Physics Laboratory, Stanford Linear Accelerator Center, and Thomas Jefferson National Accelerator Facility.

Phone: (515) 294-2635  
Fax: (515) 294-3751  
E-mail: harris@ameslab.gov

**Argonne National Laboratory**

Ms. Deborah Clayton, Manager  
SC LTR Program  
ITD-900

Argonne National Laboratory  
9700 South Cass Avenue  
Argonne, IL 60439  
Phone: (630) 252-4694  
Fax: (630) 252-5230  
E-mail: dclayton@anl.gov

**Brookhaven National Laboratory**

Mr. Michael Furey, Manager  
SC LTR Program  
Brookhaven National Laboratory  
P.O. Box 5000  
Upton, NY 11973  
Phone: (516) 344-2103  
Fax: (516) 344-3729  
E-mail: mfurey@bnl.gov

**Fermi National Accelerator Laboratory**

Mr. John Venard, Manager  
SC LTR Program  
ORTA  
Fermi National Accelerator Laboratory  
P.O. Box 500, MS 200  
Batavia, IL 60510-0500  
Phone: (630) 840-2529  
Fax: (630) 840-8752  
E-mail: venard@fnal.gov

**Lawrence Berkeley National Laboratory**

Mr. Chris Kniel, Manager  
SC LTR Program  
Lawrence Berkeley National Laboratory  
Mailstop 90-1070  
Berkeley, CA 94720  
Phone: (510) 486-5566  
Fax: (510) 486-6457  
E-mail: crkniel@lbl.gov

**Oak Ridge National Laboratory**

Ms. Louise Dunlap  
Director, Partnerships Office  
Oak Ridge National Laboratory  
P.O. Box 5000  
Oak Ridge, TN 37831  
Phone: (423) 576-4221  
Fax: (423) 576-4181  
E-mail: dunlaplb@ornl.gov

Dr. Terry Payne, Manager  
SC LTR Program

(423) 574-0008

pay@ornl.gov

**Pacific Northwest National Laboratory**

Mr. Bruce Harrer, Manager  
SC LTR Program  
Pacific Northwest National Laboratory  
P.O. Box 999, K9-21  
Richland, WA 99352  
Phone: (509) 375-6958  
Fax: (509) 375-6838  
E-mail: bj\_harrer@pnl.gov

**Princeton Plasma Physics Laboratory**

Mr. Lewis D. Meixler, Manager  
SC LTR Program  
Office of Technology Transfer  
Plasma Physics Laboratory Forrestal Campus, Rt. 1  
P. O. Box 451, M. S. 17  
Princeton, NJ 08543  
Phone: (609) 243-3009  
Fax: (609) 243-2418  
E-mail: lmeixler@pppl.gov

**Stanford Linear Accelerator Center**

Mr. Jim Simpson, Manager  
SC LTR Program  
Office of Technology Transfer  
Stanford Linear Accelerator Center  
P.O. Box 4349, MS 14B  
Stanford, CA 94309  
Phone: (650) 926-8604  
Fax: (650) 926-4999  
E-mail: jsimpson@slac.stanford.edu

**Thomas Jefferson National Accelerator Facility**

Dr. H. Frederick Dylla, Manager

SC LTR Program

Thomas Jefferson National Accelerator Facility

1200 Jefferson Avenue

Newport News, VA 23606

Phone: (757) 269-7450

Fax: (757) 269-6357

E-mail: [dylla@jlab.org](mailto:dylla@jlab.org)

**ABSTRACTS OF MULTI-YEAR PROJECTS SUPPORTED IN FY 1998****ADVANCED MATERIALS****Design of Materials**

**1. Title:** High Performance Tailored Materials for Levitation and Permanent Magnet Technologies

**ID:** ANL97-02

**PI:** George Crabtree  
Materials Science Division

**Phone:** 630 252-5509

**Partner:** Superconductive Components, Inc.  
Columbus, Ohio

**FY 98 Funding:** \$109K

**Total Project Funds:** \$750K

The objective of this project is to develop high performance bulk materials for superconducting technologies, including levitation, frictionless bearings, motors, generators, and trapped field magnets. The goal is being addressed on three levels: application of basic materials research tools and techniques to explore and understand the flux pinning mechanisms in the (RE)BCO family of superconductors, development of novel processing techniques to optimize materials performance, and integration of these techniques to produce prototype materials suitable for commercial application. The project has achieved significant successes in all three of its objectives. First, basic materials research tools such as magnetization measurements (using SQUID, vibrating sample magnetometer (VSM), and miniature Hall probes), magneto-optical imaging, and scanning electron microscopy (SEM) have revealed the materials characteristics and processing conditions leading to high performance. The project has identified processing variables, such as the high temperature growth rate, the post-growth low temperature oxygen anneal, and rare earth composition of the starting materials, which are key factors in the ultimate performance of the materials. Second, new processing techniques making extensive use of this basic research information have been developed which control the materials performance at low and high magnetic field. For example, the peak performance field can be adjusted to any value between zero and 5 Tesla. Third, new fabrication techniques have been developed which allow the manufacture of large scale monolithic components of arbitrary shape. These fabrication techniques are based on novel multiple seeding procedures and innovative joining

technology conceived and developed as part of this project. Test devices such as solenoids and rings have been fabricated and tested. In the remaining years of the project, further improvements in materials performance will be made, and simpler and more effective fabrication procedures will be developed. This project provides high performance materials for a new generation of bulk superconducting applications. The new processing allows tailoring materials to high field applications like trapped field magnets or motor components, or to low field applications like levitation or frictionless bearings. The development of monolithic fabrication procedures enables qualitatively new applications, such as motor components or shielding enclosures free of detrimental grain boundaries which limit current flow. This project supports the DOE mission to create new materials technology for the applications of superconductivity.

**2. Title: Ionically Conductive Membranes for Oxygen Separation****ID:** LBL97-03**PI:** Steven Visco  
Materials Sciences Division**Phone:** 510 486-5821**Partner:** Praxair, Inc.  
Tonawanda, New York**FY 98 Funding:** \$225K**Total Project Funds:** \$475K

The global market for industrial oxygen is estimated at about 20 billion annually. The dominant technology for the production of commercial oxygen is cryogenic distillation. The high capital equipment costs for cryogenic O<sub>2</sub> separation limits this technology to large installations. Accordingly, industrial suppliers of oxygen are highly motivated to develop technologies that can satisfy increasing demand for oxygen through smaller scale plants. One approach under development elsewhere is the use of mixed ionic-electronic ceramics. When such ceramic electrolytes are exposed to compressed air on one side and ambient pressure on the other, oxygen diffuses through the mixed conductor from the compressed side to the low-pressure side due to the chemical potential gradient of oxygen across the membrane. The drawback to this technology is the need for a compressor that raises issues of noise and reliability. Another problem is that permeation delivers ambient pressure oxygen. In



contrast, this project will use the efficient electrolytic extraction of oxygen from air using novel thin-film structures consisting of high strength ionic membranes supported on porous, catalytic electrodes. Using this technology, high purity O<sub>2</sub> can be electrochemically pressurized as an integral part of the separation process. The simplicity of operation of an electrolytic O<sub>2</sub> generator promises high reliability as well as low cost. Still, to survive as a commercial process, this approach must be cost-competitive to cryogenic production of O<sub>2</sub>. The key to success is highly efficient operation (low power consumption) of the device along with low fabrication costs. Power losses in the electrolytic oxygen cell will be related to ohmic losses across the electrolyte membrane, charge transfer polarization at the electrode/electrolyte interfaces, and mass transfer polarization across the electrodes. This project addresses the above issues in such a way that both scientific and technical success is likely. In the project, Praxair has defined performance targets for laboratory devices, while the Lawrence Berkeley National Laboratory (LBNL) team developed materials and structures for electrolytic oxygen separation. The research effort proceeded on schedule, and milestones were met as expected. The LBNL team successfully engineered laboratory O<sub>2</sub> electrolysis devices that performed at targeted performance levels, augmenting the optimism of a successful partnership. This research supports the DOE mission in materials research and applications.



**3. Title: Light Emission Processes and Dopants in Solid State Light Sources**

**ID:** LBL97-13

**PI:** Eugene Haller  
Materials Sciences Division

**Phone:** 510 486-5294

**Partner:** Hewlett-Packard Laboratories  
Palo Alto, California

**FY 98 Funding:** \$250K

**Total Project Funds:** \$750K

Light emitting diodes (LEDs) functioning in the red and infrared have been manufactured in large quantities since the 1960s. However, until very recently, only very inefficient and dim LEDs were available in the green and, especially, in the blue. Although there are a handful of semiconducting materials with sufficiently wide bandgaps to function in principle in the blue region of the spectrum,

fundamental material properties and limitations have prevented bright and efficient diodes from being made. Recently, breakthroughs in the heteroepitaxial growth of gallium nitride (GaN) and its alloys with indium and aluminum have changed the blue and green LED technology outlook. Formerly, it was believed that III-V nitride layers had too high a defect density to function as LEDs. Nevertheless, a Japanese company (Nichia) has developed a family of blue and green LEDs based on GaN that are bright and efficient. For the last three years, Japanese companies have been manufacturing and selling blue GaN LEDs in bulk quantities. This project is a collaboration with HP, the leading U.S. producer of LEDs, to investigate the fundamental light-emitting mechanism in GaN-based LEDs. HP is providing GaN and InGaN layers and structures grown with their metal-organic chemical vapor deposition (MOCVD) equipment. Joint work is being performed in four technical areas: (1) Doping related strain effects in GaN and InGaN epitaxial layers, (2) Metal/GaN contacts, (3) Localization properties of dopants and defects, and (4) Carrier transport in layers and devices. In the first technical area, it has been shown that compressive film stress and Si concentration, which were found to be positively correlated in previous work, could be varied independently by appropriate changes in growth conditions. This is of considerable importance to HP, because reliable production of thick GaN layers had been limited by cracking induced by the Si dopant. In work related to the localization and transport topics, optical measurements have been performed in diamond anvil cells with p-doped GaN single crystals, GaN, AlGaIn, and InGaIn single layers, and GaN/InGaIn multilayer structures. These results are being used to understand the mechanism of light production in III-V nitrides supporting DOE's mission in materials research.



**4. Title: Combinatorial Discovery and Optimization of Novel Materials for Advanced Electro-Optical Devices**

**ID:** LBL97-18

**PI:** Xiao-Dong Xiang  
Materials Sciences Division

**Phone:** 510 486-4864, x5315

**Partner:** NZ Applied Technologies (NZAT)  
Woburn, Massachusetts

**FY 98 Funding:** \$250K

**Total Project Funds:** \$750K

Advanced materials are the building blocks of the emerging photonic technologies which are the foundation for a new industrial base. Complex oxide ceramics (ternaries and higher order compounds) exhibit a wide range of technologically significant properties such as the electro-optic effect. The rapid expansion in the types of phenomena exhibited by modern advanced ceramics has revived interest in the use of complex oxides for advanced optical device applications. However, due to the complexity of multi-component oxides, searching for new materials or optimization for existing materials is a forbidding task for the materials community. This project will: (1) use the method of combinatorial synthesis and screening, recently developed at Lawrence Berkeley National Laboratory, to evaluate a wide range of oxide materials and compounds and optimize the advanced oxide materials for electro-optical devices; and (2) use heteroepitaxial thin film growth methods, developed at NZAT, to fabricate advanced oxide electro-optical devices based on the project's search and optimization results. In the first year, the project has developed new techniques for fabrication and syntheses of high quality epitaxial thin film material suitable for combinatorial libraries. The project has also completed the construction of the measurement system that will allow for the measurement of the electro-optical coefficient of these combinatorial libraries. This measurement system was calibrated using devices fabricated by NZAT. The goal of the project is to produce commercially viable advanced electro-optical devices. If successful, this project will play an important role in forming a strong foundation for the emerging large scale integrated optics device industry. This supports the DOE mission in materials research.



**5. Title:** Alloy Design of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  Permanent Magnets

**ID:** ORL94-15

**PI:** Joseph A. Horton  
Metals and Ceramics Division

**Phone:** 423 574-5575

**Partner:** Magnequench International, Inc.  
Anderson, Indiana

**FY 98 Funding:** \$165K

**Total Project Funds:** \$590K

The objective of this project is to improve the room temperature fracture toughness and fracture strength of neodymium based permanent magnets. Demanding motor applications, such as a prototype electric vehicle drive motor with a 150 mm diameter neodymium magnet and spun at 10,000 rpm, need an improvement in these properties to produce acceptable failure rates for commercial use. This project is one of the first studies emphasizing mechanical properties of rare earth permanent magnets. Based on a survey of commercially available material produced by two different processes, melt spinning and powder metallurgy, and a survey of experimental alloys produced by Magnequench, the project has determined that the toughness is a function of both grain size and the composition and distribution of certain grain boundary phases. Processing variables were studied to optimize magnets with Magnequench's current composition and processing methods. A third processing route utilizing gas atomized magnet powder was investigated, and bulk magnets were successfully produced. In other tetragonal intermetallics, cleavage on basal planes is often observed. Cleavage fracture surfaces in single crystals of  $\text{Nd}_2\text{Fe}_{14}\text{B}$  were analyzed by x-ray diffraction and atomic force microscopy and found to have a random orientation and some curvature. Auger electron spectroscopy analysis of the fracture surface chemistry showed that the large grained sintered materials cleave, while in the small grained-hot pressed Magnequench MQII magnets, fracture is largely intergranular. In the as melt spun material, fracture is either by cleavage or there is no grain boundary eutectic phase present. Microstructural analysis of a new grade of Magnequench powder, termed B+, was performed showing a much greater uniformity of grain size and shape through the thickness of the ribbon resulting in a magnetic powder with higher energy products. A correlation of crystallographic texture, magnetic anisotropy, press direction, microstructure, and fracture toughness is underway in order to understand the preferred directionality of some of the failure situations. This project supports DOE's basic science programs in alloy and ceramic science.



**6. Title:** The Role of Yttrium in Improving the Oxidation Resistance in Advanced Single Crystal Nickel-based Superalloys for Turbine Applications

**ID:** ORL95-07

**PI:** Edward A. Kenik  
Metals and Ceramics Division

**Phone:** 423 574-5066

**Partner:** Pratt and Whitney  
East Hartford, Connecticut

**FY 98 Funding: \$30K****Total Project Funds: \$320K**

The focus of this project is the examination of the role of yttrium and other alloying elements in the microstructure and oxidation performance of improved single crystal nickel-based superalloys for advanced turbine applications. The microstructure and microchemistry of these alloys and their surface oxides are being measured with state-of-the-art microanalytical techniques (atom probe field ion microscopy and electron microscopy) and then correlated with burner rig and engine test oxidation performance. Recent results have dealt with distribution of alloying elements between the superalloy and the oxide scale, including the formation of Ta oxides in the scale, the oxidation of near-surface HfC particles to HfO<sub>2</sub>, and the segregation of reactive elements to oxide grain boundaries. The overall technical goals include: (1) identifying the partitioning behavior of the elemental additions in these superalloys before and after burner rig and engine tests, and the effect on the misfit energy between the phases in the alloys; (2) examining the oxidation performance of these newly-developed alloys; and (3) relating the microstructural observations to the observed performance. Anticipated improvements from these modified alloys include enhanced durability in the operating environments at the high temperatures required to improve energy efficiency. In addition, the availability of alloys capable of higher temperature operation will minimize the need for expensive coatings in some applications. These alloys are primarily used for the turbine components in engines which are exposed to the most extreme temperatures. These studies are relevant to both commercial land-based (energy-production) and advanced aircraft turbines used by a wide range of U.S. industries. This project supports DOE's missions in increased energy efficiency and reduced fuel consumption.

**7. Title: Interfacial Interactions of Biological Polymers with Model Surfaces****ID:** PNL97-21**PI:** Allison A. Campbell  
Materials and Chemical Sciences Division**Phone:** 509 375-2180**Partner:** Ross Products Division  
Abbott Laboratories  
Columbus, Ohio

**FY 98 Funding:** \$248K

**Total Project Funding:** \$750K

The goal of this project is to apply state of the art methods to design, synthesize and characterize systems for adsorption experiments. Specifically, molecular beam epitaxy, chemical vapor deposition and self-assembling monolayers surfaces with controlled properties such as chemistry, topography and heterogeneity will be constructed. The project will also develop, for the first time, CVD methods for producing controlled surfaces of the biologically relevant calcium oxalate, carbonate, and phosphate systems. Biological polymers of human serum albumin, Protein G and fibrinogen will be used in the adsorption experiments. These provide excellent models in that they exhibit a range of structures, sizes, and chemistries. State-of-the-art techniques of neutron scattering and reflectometry, quartz crystal microbalance, liquid chromatography/mass spectroscopy, and atomic force microscopy will be employed to study adsorption in-situ. Information on adsorption kinetics, isotherms, and protein conformation will be obtained in real time. Finally, solid state NMR experiments will be conducted that aim to identify the specific protein residues that are interacting with the surface. This investigation will provide molecular level information on specific interactions that has not yet been obtained. To date, an in-situ quartz crystal microbalance (QCM) and screw-in flow-through cell interfaced with a syringe pump has been constructed. The absorption of fibrinogen and albumin was examined onto self-assembling monolayers attached to gold electrodes deposited onto quartz crystals. In-situ protein adsorption kinetics was examined using the QCM, and ex-situ protein adsorption amounts were determined by ellipsometry. The most significant result from this study was that the OH surface resulted in reduced fibrinogen adsorbed. This is of interest because fibrinogen is considered to be a very "sticky" protein and is difficult to keep off of surfaces. The project has identified a method for studying the adsorption/desorption of proteins on various surfaces. Two classes of binding to various weak ion exchange supports have been quantified. By studying the behavior of the proteins on the chromatographic surface, the project has obtained information suggesting possible mechanisms of protein unfolding, kinetics of the adsorption/desorption process. From the data, structural characteristics of the protein in near-physiological environments have been deduced. The project is contributing to achieving DOE's mission in fundamental science, while also providing knowledge and technology to potentially enable the development of improved materials for use in health care.



**8. Title: Improved Materials for Semiconductor Devices**

**ID:** PNL98-17

**PI:** Suresh Baskaran  
Materials Sciences Department



**Phone:** 509 375-6483

**Partner:** SEMATECH  
Austin, Texas

**FY 98 Funding:** \$125K

**Total Project Funds:** \$750K

The increasingly higher performance required of semiconductor devices has resulted in a need for new materials to reduce the capacitance between metal conductor lines (interconnects) on semiconductors. The ability of a material to reduce capacitance losses is defined by its dielectric constant, and the development of interlevel dielectric materials with much lower dielectric constants than what is currently available is the focus of considerable attention within the semiconductor industry. In addition to improving electrical performance (power consumption, signal speed, and propagation noise), such materials offer the potential of significant reductions (~\$500M annually) in fabrication costs for semiconductors. The project will develop mesoporous silica dielectric films. The controlled, highly porous structure of these films make them good candidates to obtain the types of properties the semiconductor industry is seeking in low k dielectrics. Pacific Northwest National Laboratory (PNNL) will focus on the design and synthesis of the new materials, including pore design, pore characterization, surface modification, and initial process development. SEMATECH will be responsible for extensive characterization of film performance and evaluation in relation to interconnect processing for semiconductors. SEMATECH hopes to identify low k dielectric materials capable of being utilized by its member companies in the manufacture of higher performance semiconductor devices. DOE missions will benefit through an improved understanding of mesoporous materials that also have energy-related applications in catalysis and sensing, and environmental applications in chemical separations. Experiments have been initiated to increase film thickness and minimize surface topography due to the spin coating process. Using nuclear reaction analysis and the Rutherford backscattering facility at the Environmental Molecular Sciences Laboratory, porosity was determined for surfactant-based films with a range of porosity from approximately 20% to about 60%. Ideally, from both performance and integration standpoints, films should contain high porosity with isolated pores. Therefore, PNNL researchers have also begun investigation of a synthesis approach for films with closed porosity using new soluble pore-formers.



### **Advanced Synthesis and Characterization Technologies**

**9. Title:** A Facility for Studying Micromagnetic Structures

**ID:** LBL95-12

**PI:** Howard Padmore  
Accelerator and Fusion Division

**Phone:** 510 486-5787

**Partner:** IBM  
Almaden Research Center, Dept K32/802  
San Jose, California

**FY 98 Funding:** \$300K

**Total Project Funds:** \$900K

The objective of this project is to produce a powerful and unique tool for microscopic imaging of magnetic materials, a tool which will take full advantage of the capabilities of the Advanced Light Source at Lawrence Berkeley National Laboratory, and use this tool to develop new magnetic materials for high-density information storage. The microscope is based on a full-field photoelectron emission technique, and magnetic information is extracted using a synchrotron radiation spectroscopy known as X-ray Magnetic Circular Dichroism (X-MCD). The microscope will have elemental and chemical selectivity, combined with surface sensitivity, and the ability to measure surface magnetic moments. This combination of features is unique in the array of tools currently used to study magnetic materials. IBM will use the information from the studies to advance the technology of high-density information storage, thereby assisting the development of new products such as non-volatile magnetic random access memories. The PEEM1 Microscope has been fully commissioned, and its spatial resolution has been demonstrated at 0.3  $\mu$ m. The utilization of this microscope has continued in order to develop the application of photoemission microscopy to thin film materials science. Work on understanding the dewetting of layered polymer systems has continued, as has work on surface reactions induced in the lubricated surfaces of the disc-head interface in commercial magnetic disc drives. This is leading to a better understanding of the optimization of lubricants for reduction of wear. Beamline 7.3.1 is complete and has met its goals of focused spot size and intensity. The polarization chopping system was also installed, commissioned, and is now driven from the beamline control system. The new 30 KV microscope is now working, and is being commissioned under full computer control of all functions. The project's initial work has shown the resolution to be better than 50 nm as shown by analysis of the imaging of single 100 nm gold colloid particles, and the domain structure of 18 m square iron thin film pads (passivated by a thin surface layer of SiC) has been imaged. These show excellent elemental and magnetic contrast, with complete contrast reversal with use of left/right circularly polarized light. The sample transfer system has been installed, and now the work of using the microscope to study the growth and magnetic structure of layered magnetic thin films can begin. The project supports DOE's mission to develop improved materials.

**10. Title: An Advanced Hard Carbon Plasma Deposition System with Application to the Magnetic Storage Industry****ID:** LBL98-16**PI:** Andre Anders  
Accelerator and Fusion Division**Phone:** 510 486-6745**Partner:** Commonwealth Scientific Corporation (CSC)  
Alexandria, Virginia**FY 98 Funding:** \$250K**Total Project Funds:** \$750K

The goal of this project is to develop a novel plasma deposition system used to coat computer hard disks and read/write heads with ultra-thin, diamond-like carbon films that can be implemented on an industrial scale. The project will combine the commercial and basic research strengths of CSC and Lawrence Berkeley National Laboratory respectively, to develop next-generation, filtered arc deposition equipment. The project intends to couple the plasma source and macro-particle filter to complete macro-particle suppression; improve plasma transmission (hopefully double the rate compared to present efforts); trap macro-particles within the filter; and design a compact system that can be directly plugged into existing sputter coating facilities. The system will be reasonably priced and able to coat large areas. It is anticipated that the technology developed in this project will become a key tool for next generation high-density magnetic storage media, a multi-billion-dollar market in which U.S. companies currently maintain a market leadership position. The coating system is of vital interest to the U.S. computer industry. Many of the top names in the magnetic storage industry have voiced their support for a filtered cathodic arc system for advanced carbon coating. The project supports the DOE mission in advanced materials, specifically synthesis and processing by ions and plasmas.

**11. Title: Critical Vacancy-Driven Phenomena in High Energy Ion-Implanted Silicon****ID:** ORL98-18**PI:** Tony E. Haynes  
Solid State Division

**Phone:** 423 576-2858

**Partner:** Lucent Technologies  
Murray Hill, New Jersey

**FY 98 Funding:** \$125K

**Total Project Funds:** \$750K

High energy (MeV) ion implantation is now being rapidly introduced into integrated circuit manufacturing because it promises process simplification and improved device performance. However, high energy implantation introduces an imbalance of excess vacancies and vacancy cluster defects in the near surface region of a silicon crystal, which can cause problems during subsequent processing. The objective of this project is to develop sufficient understanding of the physical mechanisms underlying the evolution of these defects and interactions with dopant atoms to enable accurate prediction and control of dopant diffusion and defect configurations during processing. By teaming Oak Ridge National Laboratory with Bell Labs and Brookhaven National Laboratory, the project has access to a suite of new, complementary capabilities for experiments and modeling that promises to elucidate the vacancy behavior. To accomplish the project's objective, a systematic method to generate large, controllable, and spatially isolated vacancy concentrations in silicon will be developed using high energy implantation. This method will permit unprecedented flexibility and sensitivity in experiments designed to measure interactions involving vacancies and vacancy clusters. The evolution of vacancy profiles during thermal treatments will be monitored by conventional techniques such as positron annihilation spectroscopy, as well as some new methods that have just been developed by this team over the last 1-3 years. For instance, the team has just demonstrated a new method to measure x-ray diffuse scattering in cross section using a submicron beam at the Advanced Photon Source at Argonne National Laboratory, as well as a method to measure vacancy cluster depth profiles by labeling them with gold atoms. For a better understanding, the experimental results will be modeled using computer simulations developed at Bell Labs. Improved physical models and simulation parameters will be derived in this project that will reduce the development time and cost for the introduction of new high energy implant processes into manufacturing. This project will directly benefit the telecommunications and microelectronics industries, and contribute to improvements in cost and performance for a wide range of high-tech products, from computers and cellular phones to digital television. This project supports the DOE mission in advanced processing of electronic materials.

**Films and Coatings****12. Title: Smooth Diamond Films for Friction and Wear Applications and Chemically Protective Coatings****ID:** ANL97-05**PI:** Alan Krauss  
Chemistry Division**Phone:** 630 252-3520**Partners:** Durametallic, Inc.  
Kalamazoo, MichiganApplied Science and Technology  
Woburn, Massachusetts**FY 98 Funding:** \$325K**Total Project Funds:** \$750K

Diamond has a number of properties which, in principle, make it an exceptional material for a large number of applications. In particular, the extreme hardness (harder than any other known material), chemical inertness (it resists attack by almost all known acids and bases), and low coefficient of friction (comparable with that of Teflon™) make it an ideal candidate for a wide range of applications involving sliding or rolling contact between moving surfaces. However, conventional diamond chemical vapor deposition (CVD) methods produce coatings with extremely rough surfaces. This roughness has limited the development of diamond film technology for tribological applications, and penetration of diamond film technology into these markets has been disappointingly slow. This project concerns the use of a process developed at Argonne National Laboratory for the production of ultra-smooth diamond coatings on rotating and sliding mechanical parts in order to reduce energy consumption, improve product reliability, and reduce toxic emissions into the environment. Films produced by this process have been shown to possess tribological properties which eliminate the problems which have so far limited the use of diamond coatings for applications involving moving parts. The work to be performed addresses adaptation of the process for the production of diamond coatings that are 10-100 times smoother than those produced by existing processes. This technology will be applied to end face mechanical seals, used to prevent the leakage of gases and liquids in equipment with rotating shafts. The benefits obtained in terms of energy savings, increased productivity, reduced maintenance, and reduced release of environmentally hazardous materials for this single application will be substantial. The technology developed will also be directly applicable

to many applications in manufacturing and transportation, in most cases with similar benefits, supporting DOE's mission for developing environmentally safe energy efficient technologies for the industrial sector.

**13. Title: Near-Frictionless Carbon Coatings****ID:** ANL98-03**Phone:** 630 252-5190**PI:** Ali Erdemir  
Energy Technology Division**Phone:** 630 252-6571**Partners:** Front Edge Technology, Inc.  
Baldwin Park, CaliforniaDiesel Technology Company  
Kentwood, MichiganStirling Thermal Motors, Inc.  
Ann Arbor, Michigan**FY 98 Funding:** \$125K**Total Project Funds:** \$750K

Numerous industrial applications involve the use of mechanical devices containing components that slide or roll against one another. The efficiency and durability of these components are often limited by the friction and wear properties of the materials used to fabricate the components. For example, Diesel Technology Company (DTC) and Stirling Thermal Motors (STM) develop advanced energy conversion systems and engine components that will contribute significantly to reducing oil imports and improving air quality by reducing engine emissions. Fuel injection systems being designed and developed by Diesel Technology for use in heavy-duty diesel engines will require tighter tolerances to run on low-lubricity fuels at higher operating pressures needed to achieve emissions and efficiency goals. Since, materials used in current fuel injection systems will not survive under these aggravated



conditions, new materials and/or coatings are needed. Similarly, Stirling engines being designed by Stirling Thermal Motors will operate under tribological conditions (e.g. speeds, temperatures, loads, and working fluids) not commonly encountered, and will require advanced materials, coatings, and lubricants to ensure long-term durability. Argonne National Laboratory has developed an amorphous coating technology (Near Frictionless Carbon - NFC) that can provide coatings with exceptionally low friction and extremely good wear properties. Argonne will work with Front-Edge Technologies (FET) to commercialize Argonne's technology for fuel injection systems and Stirling engine components being developed by DTC and STM. The objectives of this project are to: (1) advance the basic understanding of the physical/chemical and tribological processes controlling the friction and wear behavior of the new carbon films, (2) demonstrate the ability of these coatings to improve the friction and wear performance of materials and components being developed by Diesel Technology and Stirling Thermal Motors, and (3) demonstrate that the coating technology can be scaled-up to coat large numbers of components on a cost-competitive basis. If successful, the NFC technology



R&D 100 Award Winner 1998

will have a significant impact not only on the technology being pursued by DTC and STM, but also in other applications found in the aerospace, biomedical, and manufacturing sectors. It builds on expertise at Argonne in tribology, coatings, and materials characterization. This project supports DOE missions in advanced materials and sustainable environments, reducing U.S. dependence on foreign oil imports, and improving U.S. air quality. This project won an R&D 100 Award in 1998.



#### **14. Title: Next Generation Corrosion Inhibitors for Steel in Concrete**

**ID:** BNL95-12

**PI:** Hugh Isaacs  
Department of Applied Science

**Phone:** 516 344-4516

**Partner:** Grace Construction Products (W. R. Grace & Co.)  
Cambridge, Massachusetts

**FY 98 Funding:** \$74K

**Total Project Funds:** \$576K

Steel-reinforced concrete is the most widely used construction material in the world. It is almost an ideal composite, with the steel providing tensile strength and the alkaline concrete imparting passivity to the steel. However, passivity can be compromised by the ingress of chlorides from a marine environment or from de-icing salts. To address this problem, corrosion inhibitors are added to the concrete mixture, usually as simple inorganic anions (e.g. nitrite). Both the mechanism of corrosion in a concrete environment and the action of inhibition are not well understood. This project is trying to elucidate the action of corrosion and the behavior of inhibitors. The objective of the study will ultimately be to develop more effective inhibition - possibly by the use of mixed anodic/cathodic inhibitors or altering the form in which the inhibitors are added. Corrosion measurements are being made of the anodic and cathodic kinetics taking place in concrete, which describe the processes occurring with and without inhibitors. Nitrite inhibitors have been found to display different degrees of effectiveness at different stages during the development of corrosion. In sufficient quantities, the inhibitors maintain passivity. A study of the passive film structure and chemistry using x-ray techniques has shown that the oxide film present in the absence of chlorides initially has a similar crystal structure at both high and neutral pH. In contrast to behavior in near neutral solutions, at high pH the passive film does not dissolve when reduced, and can be grown to relatively high thicknesses without corrosion if the steel is repeatedly oxidized and reduced. Corrosion takes place when the chloride concentration builds up and there is insufficient nitrite present to suppress initiation of corrosion. At this point, passivity breakdown takes place with the development of pitting corrosion. A membrane develops around the corroding area due to the precipitation of the ferrous chloride and separates the low pH within the pit and the high pH solution within the pores of the concrete. Nitrite or other inhibitors must pass through this membrane to influence the corrosion, and very small quantities of nitrite reduce the dissolution rate in pits. Conditions within the membrane are similar to conditions that develop when corrosion occurs at neutral pH. Similar inhibitors to those described above are predicted to be effective in concrete. Experiments are underway to assess the behavior of new inhibitors developed by W. R. Grace. This project supports the DOE mission in materials characterization and processing.



**15. Title: Development of Buffer Layers Suitable for Deposition of Thick Superconducting  $\text{YBa}_2\text{Cu}_3\text{O}_7$  Layers by a Post-deposition Annealing Process**

**ID:** BNL98-05

**PI:** M. Suenaga  
Department of Applied Science

**Phone:** 516 344-3518

**Partner:** Oxford Superconducting Technology  
Carteret, New Jersey

**FY 98 Funding:** \$125K

**Total Project Funds:** \$750K

The goal of this project is to develop a textured buffer layer on top of a metallic substrate, e.g., a textured Ni, which is compatible with the Brookhaven National Laboratory method of fabricating thick  $\text{YBa}_2\text{Cu}_3\text{O}_7$  films, a post-deposition annealing method. In order to accomplish this, the project has started: (1) the purchase and installation of a texture measurement attachment to an existing x-ray apparatus (This makes it possible to determine the degree of the texture of the buffer layer as well as the substrate and  $\text{YBa}_2\text{Cu}_3\text{O}_7$  layers), and (2) testing of the chemical compatibility of  $\text{CeO}_2$  with  $\text{YBa}_2\text{Cu}_3\text{O}_7$  layers at the high temperature required for the formation of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  layers. A texture measuring attachment to an x-ray diffractometer was purchased and was installed such that a texture analysis of the rolled tapes, the buffer, or the superconducting films can be determined. This unit has been delivered and installed, and the process of a final acceptance of the unit is being performed. Since the post-deposition annealing process for growing thick ( $> 5 \mu\text{m}$ )  $\text{YBa}_2\text{Cu}_3\text{O}_7$  involves heat treating  $\text{YBa}_2\text{Cu}_3\text{O}_7$  precursor films in a moist atmosphere at high temperatures ( $> 725^\circ \text{C}$ ), it is important to select a buffer layer material which does not interfere with the growth of  $\text{YBa}_2\text{Cu}_3\text{O}_7$ . In order to study this, the project has initially deposited a  $\text{YBa}_2\text{Cu}_3\text{O}_7$  precursor film on a  $\text{CeO}_2$  buffered single crystalline  $\text{LaAlO}_3$  and heat treated it to form a  $\text{YBa}_2\text{Cu}_3\text{O}_7$  layer on top of the  $\text{CeO}_2$ . Note that  $\text{CeO}_2$  is a well known buffer layer which is used in conjunction with pulsed laser deposition of  $\text{YBa}_2\text{Cu}_3\text{O}_7$ . Although a significant reaction takes place between the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{CeO}_2$  layers if they are heat treated above  $750^\circ \text{C}$ , the reaction appears to be sufficiently minimized by using the reaction temperature below  $735^\circ \text{C}$ . A further study is being conducted to see the extent of the reaction, and other possible candidates for the buffer materials are being examined. If this project is successful, the superconducting tapes will be used in electrical utility systems, greatly increasing the efficiency of power transmission. This project supports DOE's mission through increased energy efficiency.



**16. Title: Nanometer Characterization and Design of Molecular Lubrication for the Head-Disk Interface**

**ID:** LBL98-10

**PI:** Miquel Salmeron  
Materials Sciences Division

**Phone:** 510 486-6704

**Partner:** Seagate Technology, Inc.  
Fremont, California

**FY 98 Funding:** \$150K

**Total Project Funds:** 465K

Information recording density in magnetic storage (hard disks) is currently increasing at an annual rate greater than 60%. In the quest for ever higher performance, the trend in the industry is toward even smaller head to disk spacing. This project will attempt to characterize and design molecular lubrication for the head-disk interface (HDI). The goal of this project is to design advanced lubricants with properties tailored for the next generation of magnetic storage devices. The read head of a hard disk "flies" within 10 nanometers of the disk surface, which is protected from damage during accidental contacts by an approximately 2 nanometer thick lubricating film. Although current film thickness is now less than the length of one lubricant molecule, industry standard characterization methods, based on optical techniques, are limited to micron-scale lateral resolution. Liquids exhibit unique physical properties when confined between surfaces separated by molecular dimensions and when spread in films of molecular scale thickness. Lawrence Berkeley National Laboratory (LBNL) has developed a scanning polarization-force microscopy technique that is applicable to ultra-thin liquid films. This is the first non-invasive technique capable of imaging the structure of liquid films with approximately 50 nanometer lateral resolution and sub-nanometer normal resolution. The unique characterization methods developed at LBNL will be used to correlate nanoscale structure and properties with microscale engineering measurements and to develop and verify the performance of optimized, tailored HDI lubricants. The techniques developed at LBNL for the nanometer scale characterization of ultra-thin liquid films and droplets will be applied to determine the actual nanoscale structure, properties, and response to local contacts of head-disk interface lubricants used in current products. Exploratory studies on advanced lubricant-overcoat systems will be carried out to identify critical performance parameters, with the final goal of designing an HDI lubricant with optimized wetting and spreading properties tailored for future generations of ultra-high density storage devices. This project supports the DOE mission in the application of basic research developments in materials sciences to new technologies.



- 17. Title: Development of High-Temperature Superconducting Wire Using RABiTS Coated Conductor Technologies**

**ID:** ORL97-02

**PI:** David K. Christen  
Solid State Division

**Phone:** 423 574-6269

**Partners:** Minnesota Mining and Manufacturing Company  
St. Paul, Minnesota

Southwire Company  
Carrollton, Georgia

**FY 98 Funding:** \$260K

**Total Project Funds:** \$750K

High-temperature superconducting (HTS) materials hold promise for greatly improved energy efficiency in a number of power applications related to the production, distribution, storage, and utilization of electric energy. This project is directed at developing a new route to the fabrication of high-temperature superconducting wires for such power applications. The approach is based upon a recent breakthrough, referred to as RABiTS (Rolling Assisted Biaxially Textured Substrates), at the Oak Ridge National Laboratory (ORNL). The approach exploits the growth of crystalline biaxially-aligned coatings on long-length oriented metal tapes that are produced by simple thermomechanical processing. The achievement of biaxial texture is essential for the transport of large, loss-free electric currents, especially in the presence of magnetic fields. In the RABiTS approach, passivating "buffer" layers are deposited by electron beam and sputter deposition, and HTS coatings are deposited by electron-beam evaporation. The project is determining the scientific and technical feasibility of making long-length coated conductors that can provide operating characteristics that are currently unattainable by electrical conductor, including present prototype HTS tapes that utilize the "power-in-silver-tube" fabrication approach. ORNL research focuses on both the simplification and optimization of oxide buffer layers on reactive metals in general, and specifically is developing a simplified ex-situ approach to the co-evaporation and processing of the superconductor coatings. Recent advances at ORNL using this approach have resulted in short-segment prototype conductors with critical current densities of over a million amps/cm at liquid nitrogen temperature. 3M is actively developing the scale-up of these techniques for the production of long-length tapes in a "continuous" process. 3M has an established experience base in high-rate deposition of many materials in manufacturing technologies, and, Southwire is the leading U.S. manufacturer of utility wire and cable and is a retailer of underground transmission lines capable of 2-5 times the power transfer into urban areas, without the need for additional rights-of-way and without significant losses to resistance. Other applications, such as power transformers, motors,

current limiters, and magnetic energy storage, are projected to produce markets of tens-of-billions of dollars per year. This project supports DOE's mission to develop high-temperature superconductors.



**18. Title: Atomic Scale Structure of Ultrathin Magnetic Multilayers and Correlation with Resistance, Giant Magnetoresistance, and Spin-Dependent Tunneling**

**ID:** ORL97-03

**PI:** William H. Butler  
Metals and Ceramics Division

**Phone:** 423 574-4845

**Partners:** Honeywell Solid State Electronics Center  
Plymouth, Minnesota

Nonvolatile Electronics, Inc.  
Eden Prairie, Minnesota

**FY 98 Funding:** \$255K

**Total Project Funds:** \$750K

Giant Magnetoresistance (GMR) and Spin-Dependent Tunneling (SDT) are two recently discovered phenomena that are providing important new insights into how spin affects the transport of electrons in materials. Both phenomena also have the potential to spark revolutionary advances in several important technologies. Both require the controlled deposition of ultrathin films. In order to realize the scientific and technological potential of these phenomena, it is necessary to relate the spin-dependent transport properties to the spin-dependent electronic structure of the deposited structures. In order to do that, it is imperative to know the deposited structures at the atomic scale because spin dependent transport is very sensitive to structure at that scale. Recent advances in electronic structure theory allow the calculation of spin dependent transport, at least for ideal thin film structures. The missing key to advancement of this field is lack of atomic scale characterization of the deposited films. This project is a close collaboration between theory and experiment. Its objective is to determine the physical, chemical, and magnetic structure of GMR and SDT films and to relate their structure to their magnetic and transport properties. In order to achieve this goal, the

project is combining a uniquely powerful set of characterization tools, (X-ray Reflection and Diffraction, Atom-Probe Microscopy, Z-Contrast Electron Microscopy with Electron Energy Loss Spectroscopy, and Electron Holography) with first principles-based computer codes that are capable of calculating the spin dependent conductivity for realistic systems. The project has characterized the growth mode of the tantalum buffer layer upon which the GMR multilayers are grown, and has related it to the process conditions. These experimental studies have been supplemented with first-principles calculations of the energetics. The project has developed sample preparation techniques that allow the utilization of atom probe field ion microscopy to image magnetic multilayer interfaces. The project has used electron holography to image the fringing fields outside magnetic memory cells. Electron energy loss spectroscopy has been used to chemically analyze the interfaces of spin-dependent tunneling systems with near atomic resolution. This project supports the DOE missions in energy efficiency and energy conservation.

**19. Title: Thin Film Thermal Barrier Coatings****ID:** PNL95-07**PI:** Edward L. Courtright  
Materials Applications Department**Phone:** 509 375-6926**Partners:** Solar Turbines Inc.  
San Diego, CaliforniaHowmet Corporation  
Whitehall, MichiganElectric Power Research Institute  
Palo Alto, California**FY 98 Funding:** \$15K**Total Project Funding:** \$830K

The objective of this project is to demonstrate the feasibility of reducing the thermal conductivity of zirconia base thermal barrier coatings with nanoscale multilayer designs. If improved thermal barriers

can be developed, both aircraft and land based stationary gas turbines can be operated at higher temperatures resulting in better efficiency and substantial energy savings, contributing to DOE's energy conservation mission. Multilayer coatings can be designed to maximize infrared reflectivity while taking advantage of the phonon scattering that occurs at interfaces. The thermal dynamic stability issues that affect durability, reliability, and life-cycle performance are being investigated. Independent thermal diffusivity measurements performed by the National Institute of Standards and Technology on coatings made of alternating layers of zirconia and alumina, developed in the project, have shown that nanoscale multilayers do significantly lower thermal conductivity compared to baseline coatings. The multilayers have also been found to retain their improved thermal performance even after extended exposure at 1200 degrees centigrade for 1000 hours or more. Adherence has been found to be substrate dependent, and such issues are currently being addressed. While the coatings appear to have good intrinsic toughness, process parameters such as deposition rate, rotational speeds, and temperature must be carefully controlled to obtain this characteristic.

**Energy Conversion and Storage****20. Title: Evaluation of Fluid Catalytic Cracking Feed Nozzles**

**ID:** ANL95-09

**PI:** Rajesh Ahluwalia  
Technology Development Division

**Phone:** 630 252-5979

**Partners:** Phillips Petroleum Company.  
Bartlesville, Oklahoma

UOP Research Center  
DesPlaines, Illinois

Amoco Corporation  
Naperville, Illinois

**FY 98 Funding:** \$185K

**Total Project Funds:** \$750K



Although the importance of feed nozzle atomization to the yield of Fluid Catalytic Cracking (FCC) units is widely recognized, quantitative data on nozzle performance is not available. This project will fill the gap in knowledge by characterizing the performance of commercial feed nozzles using state-of-the-art laser-optics instrumentation. The performance data will allow companies to select commercial nozzles that are optimal for their feeds and operating conditions. In a complementary task, a hydrodynamics model is being developed to determine the impact of atomization parameters on the overall yield of FCC units. This information will be used to design and fabricate advanced feed nozzles which will also be tested at Argonne National Laboratory. A third FCC nozzle was tested recently, while a fourth was delivered and prepared for installation. The tested nozzle was a complex multi-jet type that produced a very broad fan spray on one axis but a relatively narrow spray on the perpendicular axis. The operating map for this nozzle showed that the actual performance, in terms of air and water flow rates and pressures, was not consistent with the manufacturer's expectations. Droplet velocity data were obtained for all three components of the droplet velocity vector. The resulting data base defines the fine structure of the spray jet in terms of flow asymmetries, appearance of secondary velocity peaks, and the growth of the jet boundary. The vendors can correlate the measured structure to the design of the nozzle internals. The spray jets were completely characterized in terms of the spray angle, volume flux, 3-D velocities, and droplet size distribution for one air-water ratio. A limited number of measurements were made at a second air-water ratio for comparison. Particular attention was paid to the changes in spray structure caused by an increase or decrease in assist air. A state-of-the-art multi-component droplet vaporization model was formulated. It includes heat and mass transfer processes in the droplet and gas-phase boundary layer, equations for droplet size, velocity and position, droplet-gas phase interactions and droplet-catalyst interactions. A parametric study was conducted to calculate droplet lifetime and penetration distance as a function of droplet size, and initial droplet and gas temperatures and velocity. The calculations were performed for oil compositions representative of heavy and light feeds. The results illustrated the importance of convective heating of droplets, radiative heat transfer from hot catalyst particles, and contact heating due to collision between oil droplets and catalyst particles. The project supports the DOE missions in energy research and energy conservation.



**21. Title: Synthesis and Crystal Chemistry of Technologically Important Ceramic Membranes**

**ID:** ANL97-06

**PI:** James D. Jorgensen  
Materials Science Division

**Phone:** 630 252-5513

**Partner:** Amoco Corporation  
Naperville, Illinois

**FY 98 Funding:** \$125K

**Total Project Funds:** \$510K

Achieving the conversion of natural gas to synthesis gas (syngas) using oxygen-permeable ceramic membranes would bring vast resources of natural gas within our economic reach. This new technology depends on the development of suitable ceramic membrane materials whose performance is then demonstrated in prototype reactors. This project includes the development of suitable membrane materials, in work to be done at Argonne National Laboratory, and the construction of a prototype reactor to evaluate the materials performance and demonstrate the viability of the process, in work to be done at Amoco. A suitable ceramic membrane material based on Sr-Fe-Co-O that demonstrates the potential for the desired performance has been developed and demonstrates suitable transport properties and survivability in the reactor environment. The phases present in this material have been identified, and their compositions, crystal structures, and transport properties have been individually characterized. These studies provide an understanding of which phases are responsible for the desirable transport properties and which phases contribute to the mechanical and chemical stability. In situ neutron powder diffraction, under conditions that simulate a working reactor environment, is being used to learn how the material changes at high temperature when the oxygen partial pressure is varied over a wide range, and what structural/chemical changes are associated with degradation of the material during operation. This information will be used to optimize the synthesis and processing of the membrane material. Methods have been developed for fabricating ceramic tubes that are suitable for use in a prototype reactor. Existing laboratory and pilot plant facilities are being upgraded and modified to facilitate testing of the ceramic membranes under increasingly rigorous conditions. This will provide a valid test of the suitability of the ceramic materials for use in large-scale reactors that convert natural gas into syngas supporting DOE's mission in energy conversion and environmental quality.



**22. Title: Low Temperature Liquid Phase Catalytic Synthesis of Methanol from Synthesis Gas**

**ID:** BNL95-09

**PI:** Devinder Mahajan  
Department of Applied Science

**Phone:** 516 344-4985

**Partner:** Amoco Corporation  
Naperville, Illinois

**FY 98 Funding:** \$151K

**Total Project Funds:** \$726K

Natural gas conversion into liquid fuels is a viable option to transport remote gas. An atom-economical process is under development at Brookhaven National Laboratory (BNL) that utilizes a novel homogeneous nickel catalyst operating in a liquid phase. This catalyst allows high conversion (>90%) per pass at high reaction rates (9 g-mol MeOH/g-mol Cat. h) under thermodynamically allowed low temperature (<150°C) and low pressure (<5 Mpa). These operating conditions, unique to this catalyst system, eliminate the need for gas recycle, attain excellent heat management, and allow air partial oxidation of natural gas (catalyst being inert to N<sub>2</sub>) eliminating the cost of an air separation plant during production of synthesis gas feed. This project is aimed at developing a modified catalyst that incorporates these features and addresses the following tasks: (1) for safety considerations, develop a non-Ni(CO)<sub>4</sub> catalyst precursor, (2) establish catalyst tolerance to CO, (3) establish catalyst tolerance to H<sub>2</sub>O, and (4) transfer and install the Amoco mini pilot unit at BNL for evaluation of the catalyst in continuous mode. Previous work on this project yielded a series of ligated Ni complexes, and the unit installation was completed. The two most recent tasks to be completed under the project were: (1) selection of an optimum Modified Catalyst formulation, and (2) evaluation in the Amoco Continuous Unit that is now set up at BNL. Also, a dry run was successfully performed in the unit by the BNL Amoco team. In preparation for runs in the unit, solution homogeneity with modified catalyst formulation is being addressed. A successful incorporation of this catalyst in the Methanol Synthesis process could result in up to 40% cost reduction. This novel process would give a competitive edge to U.S. companies to transport remote natural gas, and also in the emerging commercial methanol fuel cells market in the twenty-first century. This project supports DOE's mission in energy security.



**23. Title: Thin Film Lithium Batteries**

**ID:** BNL95-11

**PI:** James McBreen  
Department of Applied Science

**Phone:** 516 344-4513

**Partner:** Power Conversion, Inc.  
Elmwood Park, New Jersey

**FY 98 Funding:** \$22K

**Total Project Funds:** \$531K

This project is focused on low cost electrolytes and cathode materials for thin film lithium ion batteries. Present commercial batteries use  $\text{LiCoO}_2$  which gives the most consistent performance and life. However, it is expensive. Lower cost materials would broaden applications beyond the present high end applications such as laptop computers and camcorders. Possible lower cost substitutes are  $\text{LiMn}_2\text{O}_4$  or  $\text{LiNiO}_2$ . Reproducibility and cycle life of these materials is a problem. In this project, Brookhaven National Laboratory has evaluated several types of  $\text{LiMn}_2\text{O}_4$  and  $\text{LiNiO}_2$  as well as mixed transition metal lithium oxides. Extensive in-situ x-ray absorption (XAS) studies were done on these materials at the National Synchrotron Light Source. This was supplemented by both in-situ and ex-situ x-ray diffraction (XRD) studies. The results of these studies were correlated with material stability on cycling. The results of tests in small lithium cells showed that the most critical parameters in determining material stability were the temperature of preparation, the stoichiometry, and the use of dopants. This project supports DOE's missions in energy efficiency and alternative energy sources.



**24. Title: New Catalysts for Direct Methanol Oxidation Fuel Cells**

**ID:** BNL95-14

**PI:** Radoslav Adzic  
Department of Applied Science

**Phone:** 203 727-2278

**Partner:** International Fuel Cells Corporation  
Windsor, Connecticut

**FY 98 Funding:** \$145K

**Total Project Funds:** \$510K

The goal of this project is the synthesis and characterization of new efficient electrocatalysts for direct methanol oxidation fuel cells and development of a basic procedure for catalyst fabrication. This will assist International Fuel Cells Corporation (IFCC) in their efforts to develop an efficient methanol fuel cell for electric vehicles. The new electrocatalysts are expected to provide the oxygen-containing species to oxidize strongly bound intermediates (poisons) in methanol oxidation, without affecting the intrinsic activity of platinum particles for methanol adsorption. The latter appears to be one of the problems with the best existing Pt-Ru alloy catalysts whose activity is still insufficient. Oxides and mixed oxides of  $\text{RuO}_2$ ,  $\text{CoWO}_4$ , and  $\text{NiWO}_4$  were synthesized and characterized using x-ray diffraction and used as a support for the Pt electrocatalyst. Samples of  $\text{RuO}_2$ -doped tungstates showed activity similar to that of the best Pt-Ru alloy-based electrocatalysts commercially available. The synthesized catalysts were delivered to IFCC for evaluation in large-area electrodes. The use of in situ infrared spectroscopy and synchrotron radiation provided data on the factors governing the activity of the catalysts and the mechanism of methanol oxidation. Further work will focus on the direct oxidation pathways of CO, the poison in methanol oxidation, tungstates, and the tungstate-based electrocatalysts by electrochemical and in-situ spectroscopic techniques. These data, together with that on the long-term testings obtained by IFCC, will provide the necessary factors for further refining and optimization of the electrocatalyst for direct methanol fuel cells for electric vehicles. Fuel cell research is a key component of the DOE mission in exploring alternative energy resources.

**25. Title: New Materials for Rechargeable Lithium Batteries**

**ID:** BNL98-04

**PI:** X.Q. Yang  
Department of Applied Science

**Phone:** 516 344-3663

**Partner:** Gould Electronics, Inc.  
Eastlake, Ohio

**FY 98 Funding:** \$125K

**Total Project Funds:** \$650K

The goal of this project is to develop new electrolyte and cathode materials for rechargeable lithium

batteries, especially for lithium ion and lithium polymer batteries. Enhancing performance, reducing cost, and replacing toxic materials by environmentally benign materials, are strategic goals of DOE in lithium battery research. This project will address these goals on two important material studies, namely the new electrolytes and new cathode materials. For the new electrolyte materials, additives, organic lithium salts, and plasticizers which have been developed by Brookhaven National Laboratory (BNL) will be evaluated by Gould Electronics for potential use in commercial battery cells. New additive compounds for lithium battery electrolytes have been synthesized by BNL. Preliminary studies of using these compounds together with lithium fluoride salt in lithium battery electrolytes are very promising. These compounds will be further studied by Gould. For the cathode material studies, the project will develop new superior characterization methods, especially in situ techniques utilizing the National Synchrotron Light Source. In situ x-ray absorption and x-ray diffraction spectroscopy will be used to study the relationship between performance and the structural characteristics of intercalation compounds such as  $\text{LiNiO}_2$ ,  $\text{LiCoO}_2$ , and  $\text{LiMn}_2\text{O}_4$  spinel. Using samples supplied by Gould, very interesting results have been collected through pilot experiments. If the research is successful, the less expensive and more environmentally friendly lithium battery materials (lithium fluoride salt for electrolyte and  $\text{LiMn}_2\text{O}_4$  for cathode) will be developed for commercial applications. This project supports the DOE mission to develop the capability to discover technologically, economically, and environmentally desirable new materials and processes, and the instruments and national user facilities necessary for achieving such progress.



**26. Title: High-Rate Zinc/Air Batteries for Consumer Applications**

**ID:** LBL94-43

**PI:** Elton Cairns  
Energy Conversion and Storage Division

**Phone:** 510 486-5028

**Partner:** Rayovac Corporation  
Madison, Wisconsin

**FY 98 Funding:** \$20K

**Total Project Funds:** \$285K

Devices resulting from the miniaturization of electronic components demand more and more energy and power from consumer batteries. While many systems require a rechargeable battery, a disposable (primary) battery is more convenient in many devices, such hearing aids. The Zn/air battery is

especially appealing for use in consumer devices because of its high specific energy, low cost, and environmentally benign components. The zinc/air button cell has enjoyed wide application in hearing-aid devices. However, the power limitation of this technology precludes its use for some applications. The use of more active electrocatalysts in the air electrode leading to improvements in the power available from the Zn/air cell will render it attractive for many other consumer applications. Five electrocatalysts were chosen for evaluation in this project: platinum (Pt), palladium (Pd), silver (Ag),  $\text{La}_{0.6}\text{Ca}_{0.4}\text{CoO}_3$  (perovskite), and cobalt tetramethoxyphenyl porphyrin (CoTMPP). Two approaches were undertaken for the evaluation of these electrocatalysts in air electrodes. In the first, electrocatalysts were applied to base electrodes containing uncatalyzed carbon, supplied by Rayovac, followed by the addition of a wet-proofing layer. The second involved direct catalyzation of carbon samples and evaluation in a Lawrence Berkeley National Laboratory (LBNL) air electrode structure. Several application techniques were developed for each of four candidate electrocatalysts: platinum (Pt), silver (Ag),  $\text{La}_{0.6}\text{Ca}_{0.4}\text{CoO}_3$  (perovskite), and cobalt tetramethoxyphenyl porphyrin (CoTMPP). Prior to evaluation, a PTFE wet-proofing layer was sprayed onto the electrode surface. Steady-state performance of the catalyzed electrodes for oxygen reduction was compared to control electrodes without catalyst but with the LBNL-added wet-proof layer. The best catalysts, Pt and  $\text{La}_{0.6}\text{Ca}_{0.4}\text{CoO}_3$ , were delivered to Rayovac for evaluation in complete zinc/air button cells. Comparisons were made between the LBNL-catalyzed carbons and the Rayovac Mn-catalyzed (RC) and the Rayovac uncatalyzed carbon (NC) in the same structure. The Pd and Ag additions to the NC carbon yielded a moderate improvement in performance over the NC carbon alone. However, these catalysts showed an order of magnitude lower performance than the RC carbon alone. The addition of Pd and Ag to the RC carbon (including the Mn) lead to significant improvement in performance over the state-of-the-art RC carbon if compared on the basis of equal catalyst loadings. This project contributes to DOE's mission in alternative energy sources.



**27. Title: Development of Zinc/Nickel Oxide Batteries for Electric Vehicle Applications**

**ID:** LBL95-27

**PI:** Elton Cairns  
Energy Conversion and Storage Division

**Phone:** 510 486-5028

**Partner:** Energy Research Corporation (ERC)  
Danbury, Connecticut

**FY 98 Funding: \$20K****Total Project Funds: \$260K**

The goal of this project is to develop a light-weight, rechargeable battery for electric vehicles. This battery uses an alkaline electrolyte, a zinc negative electrode, and a nickel oxide positive electrode. It has two major advantages over competing types such as cadmium/nickel oxide (nickel-cadmium) and metal-hydride/nickel oxide (nickel-metal hydride): it delivers more energy per unit battery mass and costs less to produce. Lawrence Berkeley National Laboratory (LBNL) has developed a novel electrolyte for the zinc/nickel oxide battery that extends its useful life to several hundred charge-discharge cycles. ERC has scaled up the LBNL laboratory model by a factor of ten and has demonstrated a similarly long lifetime. This project is developing additional improvements to lower the battery mass and to increase the ability of the electrolyte to wet the electrodes. To achieve these goals, the project is incorporating lighter wicking and current-collector materials in the electrode structures. If these efforts are successful, ERC will produce full-size electric vehicle batteries for testing. A superior zinc/nickel oxide battery could be the key to inexpensive and durable electric vehicles which will reduce air pollution and petroleum imports while creating a new growth industry. The project has identified two new problems that were compromising cell performance: electrode dehydration (particularly the nickel oxide electrode) and excessive weight of the nickel oxide electrode. Modifications to the battery were developed to correct these problems. Cell designs have been simplified and made less costly. This project supports DOE's mission in alternative energy sources and conservation.

**28. Title: Development of a Thin-Film Battery Powered Medical Device****ID:** ORL95-11**PI:** John B. Bates  
Solid State Division**Phone:** 423 574-6280**Partner:** Teledyne Electronic Technologies  
Los Angeles, California**FY 98 Funding: \$165K**



**Total Project Funds: \$650K**

The purpose of this project is to utilize Oak Ridge National Laboratory's (ORNL) solid state thin film rechargeable lithium batteries as power sources for a variety of medical devices. It has been shown from laboratory experiments that thin film batteries can be used in implantable neural stimulators, pacemakers, and defibrillators resulting in a significant reduction in size and an increase in reliability and lifetime. Under licenses with Lockheed Martin Energy Research Corporation, Teledyne Electronic Technologies (TET), in conjunction with an industrial partner, have established batch production facilities for low volume manufacturing of thin film batteries for implantable defibrillators. From measurements on a number of parallel connected large area cells fabricated at TET, it has recently been shown that the capacity and pulse performance per unit area are the same as that of small laboratory cells fabricated at ORNL. This was an obvious but important demonstration that performance scales with area, and it represents a successful transfer of technology. Presently TET is progressing with the design and construction of an in-line deposition system in order to increase their production capability. The development of high power thin film rechargeable batteries for implantable defibrillators will result in a significant reduction in the size of these devices and an improvement in their reliability. Since the batteries will last indefinitely, replacement of implanted defibrillators will no longer be necessary. It is also possible that thin film batteries of a similar size could be used in cellular telephones and other consumer electronics. This project supports the goals of DOE's Chemical Sciences program on the development of advanced non-aqueous batteries.

**INTELLIGENT PROCESSING AND MANUFACTURING RESEARCH****Intelligent Design**

**29. Title:** Automotive Underhood Thermal Management Analysis Using 3-D Coupled Thermal-Hydrodynamic Computer Models

**ID:** ANL98-14

**PI:** David P. Weber  
Reactor Engineering Division

**Phone:** 630 252-4576

**Partners:** Analysis and Design Applications Company, (adapco)  
Melville, New York

Supercomputer Automotive Applications Partnership (SCAAP)  
c/o Ford Motor Company, World Headquarters  
Dearborn, Michigan

**FY 98 Funding:** \$250K

**Total Project Funds:** \$750K

The underhood of most contemporary vehicles presents an adverse environment for the operation of sensitive components. Aerodynamic, package, and styling requirements reduce the size of the underhood compartment and the size of the front openings, while new components are constantly added in an already congested space. These trends lead to a reduction in the available underhood cooling flow and to increased temperature levels. Such levels, under adverse operating conditions, can cause the malfunction or failure of sensitive components. Early diagnosis and remedy of such potential problems during the design stage can significantly reduce the design time and cost, as well as increase the vehicle reliability. The vehicle manufacturers have recognized that it is desirable to replace the current practice of building and testing expensive prototypes with a numerical approach that can quickly and effectively analyze various designs and direct the designers toward the most efficient solution. The goal of this project is to develop and integrate thermal models for convective, conductive, and radiative heat transport, and to develop models for critical heat management system components including fan and heat exchangers. Substantial effort will be placed on improving the numerical solution algorithms for modeling the behavior of these three-dimensional thermal-hydraulics systems on state-of-the-art massively parallel computers. Extensive verification and validation of the resulting models will be performed by comparison to detailed thermal and flow measurements and

industry standard computational solutions. The development of a state-of-the-art commercial software product may be useful beyond the automotive thermal management analysis provided by this project. Applications in transportation, power generation, chemical and food processing, building and environment engineering, mechanical engineering, electronics, and the oil and gas industries can be expected. This project will also develop the ability to numerically test alternative underhood automotive configurations. As more and more electronic components are added to the engine in an ever decreasing space, the need to understand and manage the thermal loads under the hood become critical. This will reduce the necessity of costly experimentation and prototyping and result in faster time to market as well as reduce costs. This project supports the DOE mission to develop and apply advanced numerical algorithms and modeling on massively parallel computers.

**30. Title: Mathematical Simulation of Glass Production**

**ID:** PNL98-10

**PI:** George Fann  
Applied Mathematics Group

**Phone:** 509 375-6446

**Partners:** Corning Inc.  
Corning, New York

International Business Machines  
Waltham, Massachusetts

**FY 98 Funding:** \$250K

**Total Project Funds:** \$625K

A critical need exists in the glass industry to produce specialized glass products in a cost-effective manner using improved and optimized production methods. Simulation software can be used to assist the optimization of the manufacturing process by predicting the behavior of materials as well as their flow during different phases of the manufacturing process. In addition, there is a desire to model the glass manufacturing process from the viscous liquid state to the fully hardened state. However, present commercial modeling software cannot reliably meet production needs and engineering optimization requirements. The objective of this project is to develop software for massively parallel

computers that is capable of accurately simulating the various phases of the glass production process. This project will develop methods and formulations for solving free and moving boundary value problems that are encountered in simulating the flow and hardening of liquid glass during the manufacturing process. The approach is to capture multi-scale physical characteristics using a multiwavelet spectral discretization of the flow. The industrial benchmark problems are being provided by Corning. Sample problems from the materials processing groups at Pacific Northwest National Laboratory will be obtained. DOE missions will benefit through the application of the knowledge and techniques realized through the project to other efforts, such as waste vitrification using glass-like materials, as well as manufacturing of existing and new amorphous materials. The level-set method to track complicated boundary conditions will be used. A level set formulation for non-isothermal flow based on some simple assumptions has been derived. In the area of numerical methods, a new pseudo-spectral method based on wavelets for solving the flow of materials exhibiting high viscosity is being tested. In the area of computer science, a secure distributive collaborative and computing environment has been set up so that the IBM-MIT parallel real time visualization tool pV3 can be used.

**Intelligent Manufacturing Processes****31. Title: Microfabrication of a Multi-Axis Accelerometer Using High Aspect Ratio  
Microfabrication and Silicon Machining****ID:** BNL94-02**PI:** John B. Warren  
Instrumentation Division**Phone:** 516 344-4203**Partner:** Loral Control Systems  
Archbald, Pennsylvania**FY 98 Funding:** \$20K**Total Project Funds:** \$600K

The goal of this project is to use microfabrication methods developed at Brookhaven National Laboratory (BNL) to improve the performance and reduce production costs of a multi-axis

accelerometer originally constructed and tested by Loral Control Systems. In its original configuration, the accelerometer can simultaneously detect accelerations along three translational and three rotational axes; a capability that is unique for an instrumental package that has a volume of about 8 in<sup>3</sup>. The primary goal of this project is to use high aspect ratio microfabrication to bulk fabricate all of these components, thus minimizing precision machining steps and greatly reducing production cost. In addition, the inherent accuracy of the microfabrication (based on lithography) should lead to additional improvements in performance. The completed micro-accelerometer will have many commercial applications in aviation, auto navigation, active automotive suspension system control, drillbit navigation, and airbag deployment. The high aspect ratio microfabrication process is currently being used at BNL to construct prototype position-sensitive x-ray detector arrays that have many applications in high energy physics. Recently, research has concentrated on the development of high aspect ratio resists that can be adapted for levitation coil fabrication, the most cost-critical component of the sensor. It has been conclusively demonstrated that a new epoxy-based resist (SU-8, manufactured by Dupont) enables the fabrication of microstructures with aspect ratios of 15 to 1. This is an improvement of almost a factor of 3 over traditional ultraviolet based resists and is directly competitive with the traditional LIGA process (x-ray based lithography requiring synchrotron exposure). Characterization of the SU-8 resist has been completed, and data that exhaustively describe all common processing parameters have been recorded. The mechanical and electrical properties of SU-8 have been studied as well. In particular, the mechanical rigidity and dielectric constants of the material have shown that it can be incorporated into the sensor as a structural component. Of particular importance is a multi-level processing method that allows successive layers of SU-8 to be patterned to form complex three-dimensional microstructures. By metallizing each successive layer, it is possible to form multi-layers "vias" in the same fashion as a multi-layer printed circuit board. The minimum conducting line fabricated with this method can be as small as 2.5  $\mu\text{m}$ , an order of magnitude smaller than a typical copper pathway on printed circuits. This project supports the DOE missions in materials processes and electronics.



### **32. Title: Development of an Aluminum Bridge Deck System**

**ID:** ORL94-56

**PI:** H. Wayne Hayden  
Metals and Ceramics Division

**Phone:** 423 574-6936

**Partner:** Reynolds Metals Company  
Richmond, VA

**FY 98 Funding: \$95K****Total Project Funds: \$800K**

The purpose of this project is to develop and eventually commercialize an aluminum bridge-deck panel system based on the use of aluminum multi-void extrusions which are welded to make panel sections and coated with an aggregate/epoxy composite as the pavement wear surface. The panels are then bolted in place to existing bridge sub-structure. Work at ORNL has concentrated on critical issues affecting the performance life of decks under projected conditions of loading and exposure temperature. ORNL studies during the first year demonstrated acceptable fatigue lifetimes of bolted joints; no undue residual-stress development in the vicinity of welds; non-destructive evaluation (NDE) procedures for weld and pavement surface bonding; and the role of monotonic and fatigue loading on delamination of the wear surface. ORNL studies are now concentrating on establishing tensile stress and interfacial shear-stress limits for the wear surface/aluminum bond and fatigue loading behavior of welded sections. The desired results are to begin the upgrade of deficient bridges throughout the U.S. with the use of aluminum bridge decks, and to use aluminum decks on new bridges. Two replacement bridge decks, one in Pennsylvania and one in Virginia, using the Reynolds decks, are now in operation and are generating interest from many state highway departments as well as many non-US concerns. This project clearly enhances DOE missions in transportation technology, infrastructure, energy conservation, and environmental quality.

**33. Title: Rapid Prototyping of Ceramics****ID:** ORL94-95**PI:** Robert J. Lauf  
Metals and Ceramics Division**Phone:** 423 574-5176**Partner:** Performance Research  
Denver, North Carolina**FY 98 Funding: \$175K****Total Project Funds: \$634K**

Ceramic components, especially those with complex shapes, are costly to manufacture and require long lead times to develop tooling for forming. The goal of this project is to develop fundamental

knowledge regarding novel approaches for rapid fabrication of ceramics. This project is investigating rapid prototyping techniques, such as stereolithography, masked layer assembly, and laser ablation of green ceramics. Key to their successful application will be the creation of appropriate computer data files. The objective is to identify a novel, yet feasible, approach to rapid ceramic component prototyping and to demonstrate the technique by fabricating complex-shaped hardware directly from computer files. Successful accomplishment of these research goals will enable rapid fabrication of complex-shaped ceramic components. The potential energy-related applications are numerous and varied, and include automotive and aerospace heat engine components, biomedical devices, electronics manufacturing equipment, and many other industries. The project has demonstrated file conversion from a CAD drawing file to a computer control code for building a component on the 3D Systems stereolithography apparatus (SLA). Resin casting molds were fabricated directly from drawings, and ceramic components were gelcast in the molds. The project has identified software for converting medical Computed Tomography and Magnetic Resonance Imaging (MRI) data to SLA files. Ultraviolet (UV) curing agents have been tested with gelcasting slurries and have been shown to form excellent gelled bodies. This curing system is being evaluated for use in the SLA to substitute a ceramic slurry for the normal liquid resin to form sinterable green ceramics directly on the SLA. The UV-cured gelcasting slurry is also being evaluated for masked layer assembly (MLA) fabrication. In the MLA system, a series of computer-generated masks is used to selectively cure successive layers and build a 3-dimensional solid object from a liquid slurry. Unlike the SLA system which writes each layer using a laser point source, in the MLA system an entire layer is cured by a single exposure to an UV flood lamp. Using the MLA system, total build time is unaffected by the complexity of individual layers. Evaluation of a third rapid prototyping method, laser ablation (LA), has begun. Using LA, the organic binder holding together the ceramic particles in an unfired gelcast ceramic is selectively ablated using a computer-controlled laser. A subtractive process thus produces a complex shape. Ceramic samples have been sent to a laser system manufacturer for testing of the feasibility of this process. This project supports DOE's efforts in advanced manufacturing and ceramics.



**34. Title: Neural Networks for Metal Forming Die Design**

**ID:** ORL95-90

**PI:** Thomas Zacharia  
Metals and Ceramics Division

**Phone:** 423 574-4897

**Partner:** Lear, Inc.  
Morristown, New Jersey

**FY 98 Funding: \$176K**

**Total Projects Funds: \$905K**

The highly iterative nature of the die design process constitutes both a technical and an economic limitation on the effective utilization of industrial sheet metal forming methods. The goal of this project is to minimize these limitations. This required development of a method for generating "Inverse" solutions from data representing a "Forward" problem. Modeling codes exist with which one can compute material deformation in response to a specified "tooling" configuration (the "Forward" problem). The objective was to use the "Forward" results of computational modeling to support a method for automatic generation of die designs. The data generalization and codification capabilities of Artificial Neural Networks made them a natural choice for solving the Inverse problem. Because such networks do perform well with the large, two-dimensional data sets required for die and component shape definition, a major objective of the project was development of methods for representing three-dimensional surfaces sparsely. Recent work has involved refining an earlier-developed data compression method ("Patch Method") for representing the (often) subtle shape differences between a desired component and the tooling that would produce it under specified stamping conditions. Prior to its development, computer memory requirements permitted network training with no more than twenty data sets. Training sets now include eighty members and, with presently anticipated improvements, should include more than two hundred. Equally important are the network algorithm modifications that have led to nearly one order of magnitude reduction in rms die shape prediction error. The general applicability of the "Patch Method" was demonstrated when a network trained to generate die designs only for "pan-like" and "tophat-like" shapes was able to produce a reasonable first-pass design for an elliptical shell component for which no training examples had been presented. Thus, the network appears able to learn general and broadly applicable deformation relationships, not only geometry-specific ones. Attention is now focused on completion of a graphical user interface. If, as expected, the developed method leads to the reduction of even one iteration of a typical die design process, the potential savings can amount to billions of dollars per year. Because, the Patch/neural network method appears to be a very general one, it should be applicable to any industrial process for which the ability to capture relationships in three-dimensional data is important. This project supports the DOE mission to develop a real-time tool that can capture the predictive capability of the most sophisticated, validated computational tools for process control and tooling design.



**35. Title: Fabrication of Cast Metal Matrix Components****ID:** ORL95-01**PI:** James R. Hansen  
Engineering Technology Division**Phone:** 423 241-2102**Partner:** Metal Matrix Composite Castings  
Waltham, Massachusetts**FY 98 Funding:** \$70K**Total Project Funds:** \$760K

The goal of this project is to produce low cost, high quality (pore free) metal-matrix composite components via a high production rate process. The approach is to pressure cast near-absolute net-shape components by using inexpensive, nonstructural tooling. Metal matrix composite components are manufactured by first forming a ceramic preform and then infiltrating the preform with molten aluminum alloy using Metal Matrix Cast Composites (MMCC) patented pressure-infiltration casting technology. The overall objective is to demonstrate cost-effective manufacturing technology on composite material with the strength and stiffness of cast iron and the weight of aluminum. Critical tasks are to tailor gelcasting process parameters and slurry rheology to enable the fabrication of defect-free preforms from MMCC specified powders for a low-cost manufacturing process, demonstrate inexpensive tooling, characterize the mechanical behavior of metal matrix composites, and evaluate the performance of a brake caliper. This project supports DOE programs by developing technology to manufacture lightweight automobile parts, thereby reducing vehicle energy consumption. The high production rate of pressure cast composites can dramatically increase introduction of metal matrix composites into the automotive market. The immediate application of the technology is to automobile brake components. For example, by replacing a Lincoln Town Car's cast-iron brake calipers with aluminum matrix composite, the total brake caliper weight is reduced by 60% with no loss of stiffness. Project accomplishments include: (1) tailoring ORNL's patented gelcasting technology to produce preforms packed to about 50% by volume with inexpensive alumina particles; (2) developing slurry rheology to produce stable gelcasting slurries that avoid particle settling problems; (3) developing mold releases that eliminate adherence of a gelcast preform to mold walls; (4) demonstrating techniques for filling simple molds with a patented hydraulic-casting apparatus; (5) designing nonstructural tooling and using it to manufacture calipers with excellent surface finish and dimensional control; (6) evaluating numerous batches of cast composite material by modulus of rupture, tensile, and fracture toughness tests and modeling with constitutive theories; and (7) fabricating a test fixture and testing a metal matrix

composite caliper along with a reference cast-iron caliper. The project has demonstrated that metal matrix composite brake calipers manufactured via pressure infiltration casting have the stiffness of cast iron and the weight of aluminum. This development should lead to rapid expansion of these lightweight composite materials into the automotive brake industry and bring about improved automobile efficiency.



**36. Title: Controlled Nonisothermal Hot Forging Using Infrared for Microstructural Control**

**ID:** ORL98-08

**PI:** Craig A. Blue  
Metals and Ceramics Division

**Phone:** 423 574-4357

**Partners:** Forging Industry Association  
Cleveland, Ohio

United Defense, LP  
Anniston, Alabama

Finkl & Sons Co.  
Chicago, Illinois

Scientific Forming Technologies Corporation  
Columbus, Ohio

**FY 98 Funding:** \$226K

**Total Project Funds:** \$450K

Hot forging is a widely used method for making metal parts from automobile and aircraft components to hand tools. Forging is a plastic deforming of metal into desired shapes by compression, usually with one or more dies to control the shape. Forging is a \$50 billion industry in the U.S. and employs 400,000 people. The heating of metal pieces prior to forging consumes large quantities of energy. Current heating practices require that an entire billet be heated to a uniform temperature prior to forging, even though only a portion of that material requires heating to that high temperature to achieve the desired plastic deformation. The goal of this project is to demonstrate the use of infrared

heating to achieve controlled local heating of steel forging billets to permit forging with reduced heating requirements and with improved control of properties in the finished part. Infrared heating makes use of quartz halogen lamps to provide rapid radiant heating of metal surfaces in an easily controlled manner. This provides the means for controlled rapid local heating superior to heating methods currently used in the forging industry. In this project, experimental studies of the heating and forging processes will be combined with computer modeling of the process to demonstrate the application of this new technology to a variety of forging applications. These include forging restrikes in which the forged part is rapidly reheated and immediately forged again to produce more complex shapes which are not now forged economically. The structure and properties of material forged with this new method will be characterized. The results will be incorporated into the computer models currently in widespread use in the industry so that optimal forging conditions, and cost and energy benefits, can be predicted for each new part. The development and use of this technology will result in reduced manufacturing costs for a wide range of consumer goods. It will also reduce energy consumption in the forging industry resulting in lower consumption of fossil fuels and less emission from electric power generating plants. This project supports DOE's mission to develop energy efficient industrial processes.

**Enabling Technologies****37. Title: Development of an In-Situ Scanning Surface Profiler**

**ID:** BNL95-07

**PI:** Peter Z. Takacs  
Instrumentation Division

**Phone:** 516 344-2824

**Partner:** Continental Optical Corporation  
Hauppauge, New York

**FY 98 Funding:** \$148K

**Total Project Funds:** \$357K

The goal of this project is to extend the capabilities of the Long Trace Profiler (LTP) to develop a new surface profiling instrument that can be used to measure the distortion produced in x-ray mirrors

exposed to high power synchrotron radiation (SR) beams. The standard LTP is used to measure the shape of mirrors in a controlled, stable laboratory environment. The new system will be able to measure mirrors in-situ as they are exposed to the high heat loads from powerful x-ray beams generated by third-generation SR sources, such as at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL) and at SPring8 in Japan. The In-Situ LTP (ISLTP) will provide valuable information to SR beam line scientists to enable them to utilize the powerful x-ray beams in the most efficient manner. A prototype system was built and tested on a beam line at the APS at ANL in late 1997. The instrument performed extremely well and discovered significant distortion effects produced on the mirror by the SR beam. This distortion had not been predicted by the finite element design codes. The success of the initial ISLTP tests at the APS has led to a request from National Synchrotron Light Source (NSLS) scientists to construct another ISLTP for use at the NSLS. The project was extended for one year to accommodate this request. Recent contacts with scientists at synchrotron facilities in Taiwan and Japan are expected to lead to further commercial development of the ISLTP instrument. The development of the LTP support instrumentation program for material sciences is a critical DOE mission area.



**38. Title: Development of Multi-Channel ASICs for CdZnTe Gamma Detector Arrays**

**ID:** BNL97-06

**PI:** Paul O'Connor  
Instrumentation Division

**Phone:** 516 344-7577

**Partner:** eV Products Division of II-VI, Inc.  
Saxonburg, Pennsylvania

**FY 98 Funding:** \$191K

**Total Project Funds:** \$652K

This project is applying new microelectronics technology developed in support of DOE's high energy physics program to solve a problem in industrial/medical imaging. eV Products is a manufacturer of Cadmium Zinc Telluride (CZT) array detectors for X and gamma rays in the 20 - 150 keV energy range. These are the only solid-state detectors available for this energy range, and as such play an important role in systems where size and weight are important requirements. To enhance the

attractiveness of CZT arrays, the front-end electronics must also be miniaturized. Up to now, eV Products has been producing detectors with hybrid circuit readout electronics. These hybrid circuits occupy an area of about 2 square inches for each channel. By implementing the electronics functions as an application-specific integrated circuit (ASIC), the project expects to provide a 16-channel readout on a single chip measuring 5 mm on a side. Several custom chips, tailored to the needs of eV Products, will be developed in the project. To date, the project has successfully coupled an existing Relativistic Heavy Ion Collider (RHIC) chip to a CZT array, and designed a new ASIC in 1.2 micron CMOS for use with eV's general purpose imaging array. The project has recently obtained very good test results with a CZT detector coupled to the CReV1 preamplifier and operated in the photon counting mode. A second prototype will be designed in 0.5 micron CMOS and fabricated by the end 1998. There is a large need for solid state gamma and x-ray imaging capability for both medical and industrial applications. Solid state CZT arrays with ASIC readouts can form the basis of a portable nuclear medicine camera, a hand held interoperative probe for cancer surgery, bone densitometry scanners for the detection of osteoporosis, explosives detectors for security screening, and high speed defect imagers for manufacturing lines. The ASICs developed in this project can also benefit the DOE mission areas of time-resolved x-ray crystallography, nuclear medicine, and extended x-ray absorption spectroscopy.



**39. Title: Microcircuits and Sensors for Portable, Low-Power Data Collection and Transmission**

**ID:** BNL97-07

**PI:** Paul O'Connor  
Instrumentation Division

**Phone:** 516 344-7577

**Partner:** Symbol Technologies, Inc.  
Holtsville, New York

**FY 98 Funding:** \$243K

**Total Project Funds:** \$750K

The goal of this project is to produce an inexpensive single-chip frequency agile radio frequency (RF) transceiver operating in the 2.4 GHz range - a universally accepted unlicensed band - with data rates

up to 250 kbps and an approximate range of 50 feet. This "radio on a chip" can play an important role in cost reduction in Symbol Technologies' existing wireless data terminal product line and offers the possibility of lightweight, cordless bar code scanners. The goal of this project is to achieve acceptable RF performance from standard industrial CMOS technology. The project has demonstrated progress towards that objective by successfully fabricating several critical circuit blocks of the transceiver in 0.5 micron CMOS. These include a fully integrated transmitter based on a phase-locked loop frequency synthesizer. This project has also demonstrated a live wireless link between a scanner, retrofitted with one of our transmitter chips, and an existing Symbol wireless data terminal, operating over a distance of up to 60 feet. Error-free transmission was obtained at a data rate of 19.6 kbps. A direct-conversion receiver has been designed, and fabrication is almost complete. Next, the new 0.35 micron CMOS technology will be investigated, which should improve the speed/power performance of the circuits. The project will design and test a low noise amplifier (LNA), a frequency-hopping synthesizer, an improved baseband receiver, and a digital signal processor (DSP) for baseband processing. Small, inexpensive radio transceivers may have a broad benefit to DOE programs in large detectors used in high energy physics colliders, where many thousands of subdetector elements need to communicate; in wireless networks which will allow data collection from remote or hazardous areas; and in providing a means for mobile access to large databases.



**40. Title: A High Resolution Subsurface Electromagnetic Imaging Tool**

**ID:** LBL94-14

**PI:** Ki Ha Lee  
Earth Sciences Division

**Phone:** 510 486-7468

**Partner:** Western Atlas Logging Services (WALS)  
Houston, Texas

**FY 98 Funding:** \$72K

**Total Project Funds:** \$545K

The goal of this project is to develop and apply a new survey method and instrumentation for high-resolution subsurface electromagnetic (EM) imaging. The technology is critically important in assisting improved management of petroleum reservoirs for increased oil production. The basis of

the technology is the new tomographic imaging technique via wavefield transform developed at Lawrence Berkeley National Laboratory (LBNL). The theoretical basis of the wavefield transform has been known for some time, but Lee et al (1989) generalized it to include EM fields and demonstrated the usefulness of such a transform using a forward model study. In that study, wavefields are first obtained by numerical modeling and corresponding EM fields are calculated by simple integration of these wavefields. Effort in the project has focused on solving the inverse problem in which a diffusive EM field is transformed to a wavefield. The velocity of the wavefield is inversely proportional to the square root of the electrical conductivity; therefore, velocity mapping directly leads to conductivity imaging. Once fully developed, the technique could produce electrical conductivity images with a spatial resolution equivalent to that of the seismic imaging for the elastic parameters. This technology will enable WALs to use the current state-of-the-art knowledge in underground imaging for increased production to the U.S. oil industry. This will directly help reduce U.S. energy dependence on foreign oil. The project supports DOE's mission in enhanced U.S. energy security. In the project, wavefield transform software was prepared and delivered to WALs. The wavefield transform concept has been verified in a laboratory model study (1-dimensional). WALs is investigating integration of LBNL's prototype transmitter for subsurface measurement. For high accuracy measurements, extensive noise suppression and application of state-of-the-art electronics are required; this was time-consuming but progress has been successful.



**41. Title: In-Line Sensors for Electrolytic Aluminum Cells**

**ID:** ORL95-04

**PI:** Jack P. Young  
Chemical and Analytical Sciences Division

**Phone:** 423 574-4922

**Partners:** Alumax Corporation  
Ferndale, Washington

Kaiser Aluminum and Chemical Company  
Pleasanton, California

Reynolds Metals Company  
Muscle Shoals, Alabama

**FY 98 Funding: \$80K****Total Project Funds: \$370K**

The objective of this project is to develop in-line sensors for commercial aluminum electrolytic cell operation. The sensors to be developed will be of a Raman spectral type. The research goal is to develop technology which will allow measurement of soluble alumina, bath ratio, and bath temperature. These in-line measurements will be inputs to new process control algorithms that can then be developed to improve the efficiency of aluminum electrolysis operations thereby reducing energy consumption. Such energy saving is in line with the goals of DOE. The improved control algorithm will also lead to a reduction in the anode effect which results in wasted energy and fluorocarbon emission. Reduction of potentially hazardous environmental gases is also a goal of DOE. Progress has been made in achieving these goals. Short-term compatibility tests of several candidate sheath materials have been carried out. Longer term tests are being conducted by Kaiser Aluminum and Chemical and Reynolds Metals. By a modified Raman spectral approach, the concentration of soluble  $\text{Al}_2\text{O}_3$  in cryolite mixtures has been measured in molten or solid samples. Raman studies of fluor-aluminum species in cryolite melts are also underway using this approach.

**42. Title: An Implantable, Incipient Failure Monitor for Use in Roller-Cone Oil-Field Drill Bits****ID:** ORL95-13**PI:** David E. Holcomb  
Instrumentation and Controls Division**Phone:** 423 576-7889**Partners:** Hughes Christiansen  
The Woodlands, TexasHouston Advanced Research Center  
The Woodlands, Texas**FY 98 Funding: \$95K****Total Project Funds: \$680K**



The purpose of this project is to develop an incipient failure prediction system that can be incorporated into production roller-cone, oilfield drill bits. Catastrophic drill bit failure is an expensive problem in the petrochemical well drilling business. The cost of catastrophic bit failure (loss of cones) can exceed \$1 million per well (worst case ~\$5.5 million). On an annual basis, industry costs for bit cone loss range from \$30 to \$60 million. To avoid these failures, bits are typically replaced with significant remaining life. The costs associated with replacing a single bit can exceed \$100 thousand. The technical approach chosen to solve this problem was to: (1) determine a drill bit parameter characteristic of incipient failure; (2) design and fabricate instrumentation implantable directly into drill bits to record the failure signature, make decisions about impending failures, and initiate communication to the surface; and (3) develop a signaling to the surface communication link. Bearing lubricant impedance was selected as the parameter indicative of incipient failure. Laboratory testing of returned failed bits enabled the establishment of the failure criteria. Impending failure is communicated to the surface by altering the pressure drop across the bit body by opening an additional mud flow nozzle. Novel electronics have been designed and fabricated and are in the process of being field tested and optimized to allow simultaneous measurement of the lubricant condition within each bit journal bearing. The electronics assembly is required to be: highly dense (to fit within standard drill bit bodies), high temperature tolerant (to withstand ambient downhole temperatures), low power (battery powered for throughout the life of the drill bit), and highly vibration tolerant. A novel impedance recording circuit was developed which does not require absolute signal levels to obtain temperature. Four channels of the circuit (along with signal conditioning electronics) were compressed into an ASIC (application specific integrated circuit) along with the logical (digital) components of the impedance logging scheme. The remaining project tasks are extensive field testing of the developed system, and transferring the electronic module manufacturing and assembly technology from Oak Ridge National Laboratory to Hughes Christensen. This project supports two DOE missions. First, the project reduces the cost of oil well drilling, increasing achievable U.S. domestic petroleum production and thereby reducing the national strategic dependence on imported oil. Second, this project increases the international competitiveness of a U.S. manufacturer subject to aggressive foreign competition, helping to preserve U.S. manufacturing jobs.



**43. Title: Microfabricated Instrumentation for Chemical Sensing in Industrial Process Control**

**ID:** ORL97-08

**PI:** J. Michael Ramsey  
Chemical and Analytical Sciences Division

**Phone:** 423 574-5662

**Partner:** Waters Corporation  
Milford, Massachusetts

**FY 98 Funding:** \$260K

**Total Project Funds:** \$747K

The goal of this project is to demonstrate microinstruments that can be used for continuous "real-time" monitoring of liquid borne chemical species in industrial process control settings. The monitoring and control of chemical constituents may be of importance for product quality control or, in the case of process effluents, of environmental concern. The project is attempting to demonstrate the use of microfabricated fluidic structures pioneered at Oak Ridge National Laboratory, referred to as "lab-on-a-chip" devices or microchips, that accomplish chemical measurement tasks that emulate those performed in the conventional laboratory. A microchip device that accomplishes the task of monitoring critical species in water must monolithically integrate filtration structures to eliminate clogging, solid phase extraction elements for sample complexity reduction and concentration enhancement, and chemical separations capability for species identification. The devices envisioned could be used as hand portable chemical analysis instruments where samples are analyzed in the field or as emplaced sensors for continuous "real-time" monitoring. Chemical separations on microfabricated structures have been demonstrated with performance that exceeds that provided by conventional laboratory instrumentation. These separations are typically two orders of magnitude faster than conventional separations technology while retaining or exceeding resolving power performance. Solid phase extraction in microfabricated structures have allowed concentration enhancement approaching two orders of magnitude. Additionally, the project has fabricated filtration functional elements for the exclusion of particulate matter. This inlet structure has been used to demonstrate the ability to autonomously sample aqueous materials external to the microchip devices using electrokinetic transport means. Solid phase extraction materials have also been synthesized and tested, using conventional stationary phase supports, for enhanced and selective extraction properties. Tasks which remain include testing of filtration elements for efficacy in elimination of particles and sampling efficiency, increased solid phase extraction efficiencies, and device integration of the independent functional elements. The resultant technology will have broad application to industrial environmental monitoring problems such as monitoring municipal water supplies (the target initial demonstration), waste water effluent from industrial facilities, or run-off from agricultural activities. Successful implementation of these microchip devices will reduce monitoring costs while enhancing performance by allowing a greater number of analyses to be performed per unit time at an array of locations. This technology development activity supports DOE's environmental remediation activities and the Industries of the Future initiative.

**44. Title: Wireless Luminescence Integrated Sensors****ID:** ORL98-09**PI:** Michael L. Simpson  
Instrumentation and Controls Division**Phone:** 423 574-8588**Partner:** Perkin Elmer Corporation  
Norwalk, Connecticut**FY 98 Funding:** \$250K**Total Project Funds:** \$750K

This project will result in the development of a family of wireless, single-chip, luminescence-sensing devices that will solve a number of difficult distributed measurement problems in areas ranging from environmental monitoring and assessment to high-throughput screening of new therapeutic drug candidates. These wireless luminescence integrated sensors (WLIS) will consist of a chip-based, low-level light sensor, wireless data transmitter, and radio frequency power input circuit all realized in a standard integrated circuit process. The project will also develop a rugged thin-film protective coating for the WLIS devices that will allow a bioluminescent or chemiluminescent compound or organism to be deposited directly on the WLIS device. While the WLIS devices will interface with a large number of luminescent (or fluorescent) assays, this project will develop and interface with bioluminescent bacteria that have been genetically engineered to be sensitive to environmental pollutants. As a model system, the project will interface the WLIS device to *Pseudomonas Putida* TVA8, a novel engineered bacteria sensitive to the environmental pollutants benzene, toluene, ethylbenzene, and xylene (BTEX). Additionally, bioluminescent cells sensitive to environmental estrogens (which are believed to adversely affect human health) will be developed and interfaced to WLIS devices. Perkin Elmer will commercialize WLIS devices as environmental sensors and as high throughput screening instrumentation used in the search for new therapeutic drugs. This project supports the DOE mission to develop a cleaner environment, improve healthcare, and locate new domestic oil and natural gas sites.

**ENVIRONMENTAL AND BIOMEDICAL RESEARCH****Biotechnology**

**45. Title: Peptide Nucleic Acid Arrays and Fluorescence Resonance Energy Transfer to Identify and Enumerate Microorganisms in Environmental Samples**

**ID:** PNL97-11

**PI:** Darrell P. Chandler  
Environmental Microbiology Group

**Phone:** 509 376-8644

**Partner:** PerSeptive Biosystems  
Framingham, Massachusetts

**FY 98 Funding:** \$250K

**Total Project Funds:** \$750K

This project contributes to DOE's environmental quality and nonproliferation missions by enabling the detection of specific bioremediative and/or pathogenic microorganisms in environmental samples (soil, sediment, sludge, groundwater, wastewater, and aerosols). The transfer of current nucleic acid purification and detection technologies to real-time environmental sample analysis are hampered by the time and expense of nucleic acid purification and the coextraction of environmental contaminants (such as humic acids) that interfere with enzymatic processes such as polymerase chain reaction (PCR) and fluorescence detection in the visible wavelengths. These limitations are being addressed by employing the novel properties of peptide nucleic acids (PNA) as a nucleic acid affinity purification reagent in a novel automated sample processing system, and as a detection reagent within the context of oligonucleotide arrays and flow-through fluorescence detection technologies. The project has examined the solution-phase binding characteristics of PNA and bis-PNA probes in crude environmental extracts and pure solutions to elucidate and understand the relationships between PNA probe size, buffer composition, salt concentration, target size, target concentration, hybridization time, and elution temperature relative to the behavior of a DNA oligonucleotide under identical solution conditions and within the context of sample preparation. The project has determined that PNAs and bis-PNAs are effective nucleic acid purification reagents within crude environmental extracts and are now coupling PNA probes to the surface of PerSeptive Biosystems' microbeads for evaluating on-line nucleic acid capture efficiency from crude environmental sample extracts. The project has validated the affinity purification concept and renewable microcolumn technology with

oligonucleotide probes coupled to a polystyrene support matrix. On-line, automated capture experiments with low concentrations (to 1 attomole) of target in a competitive genomic background of ca.  $10^9$  cells have been performed. Purification/recovery efficiencies comparable to benchtop procedures with similar soil/biomass samples have been achieved. Nucleic acid purification/concentration in the automated system was achieved in 20 minutes with 6-30% recovery efficiency, whereas the comparable benchtop procedure required 260 minutes and resulted in a maximum of 2% recovery. More importantly, nucleic acids processed in the automated system were sufficiently pure for direct PCR analysis. Due to the unique binding properties of PNA, a second generation renewable column flow cell was constructed that incorporates temperature control, and this column will be used exclusively for PNA-microbead purification of nucleic acids described above. A nucleic acid sample processing module with PNA probe technology that is interfaced directly with advanced, miniaturized thermal cyclers and other fluorescence-based detectors will be developed.



**46. Title: Microorganism Detection and Characterization**

**ID:** PNL98-03

**PI:** Darrell P. Chandler  
Environmental Microbiology Group

**Phone:** 509 376-8644

**Partner:** Genometrix Inc.  
The Woodlands, Texas

**FY 98 Funding:** \$125K

**Total Project Funds:** \$750K

Rapid and accurate detection of microorganisms is important in a number of health-related and environmental applications, such as food safety, wastewater treatment, disease diagnosis, forensics, and bioremediation monitoring. Recently, genosensor technology has been developed within the context of clinical diagnostics to detect up to  $10^6$  *different* gene targets simultaneously. Such technology has the potential to significantly improve microorganism detection and characterization in environmental samples. However, the widespread application of this technology has been limited by the costs and time required for sample preparation and analysis. The objective of this project is to develop a versatile, fully integrated, automated, high throughput gene-based detector for broad

application in health related and environmental fields. Pacific Northwest National Laboratory is utilizing its expertise in nucleic acid extraction and characterization from environmental samples, micromachining technology, and microfluidic systems and combining them with proprietary, patented nucleic acid concentration principles, surface chemistries, and detection arrays from Genometrix. The project is directed towards the development of a prototype, integrated detector that can be further enhanced by Genometrix for commercial application, while also contributing to achieving DOE mission objectives in biological research and environmental remediation. The project's first objectives include the synthesis and testing of novel microbead matrices and surface chemistries for their nucleic acid binding properties within several crude environmental nucleic acid extracts (aerosol, wastewater, soil, subsurface sediment), and applying a low-density genosensor array for the quantitative analysis of microorganisms in an industrial wastewater processing stream. These experiments will represent the first proof-of-principle genosensor detection of microorganisms from crude environmental samples and provide the technical/conceptual foundation for physically coupling a nucleic acid purification module directly to a genosensor array/reader for point-of-use devices for health-related and environmental applications.



### Medical Technologies

**47. Title: Development of Rapid Prototyping Technology for Bioceramic Applications**

**ID:** ANL95-08

**PI:** William A. Ellingson  
Energy Technology Division

**Phone:** 630 252-5068

**Partner:** Zimmer, Inc.  
Warsaw, Indiana

**FY 98 Funding:** \$95K

**Total Project Funds:** \$810K

The problem being addressed in this project is the overall reduction of medical costs of orthopaedic implants through use of advanced ceramic fabrication technology using a Solid Freeform Fabrication also called Rapid Prototyping. By using this technology, it is possible to tailor the near surface

porosity, as well as the material composition, such that the engraftment time is minimized. The objective of this project is to demonstrate that 3D x-ray computed tomographic images (CAT scan images) coupled with advanced computer controlled fabrication technology using rapid prototyping utilizing carefully prepared ceramic materials, can be used to produce implantable orthopaedic devices. The approach being followed has several parts. First, 3D x-ray image data sets are collected using a special 3D x-ray imaged device at Argonne National Laboratory. Second, special ceramic materials are developed such that when used in conjunction with the rapid prototyping machine, ceramic components can be fabricated. The fabricated bones or bone segments are inserted into cadavers, the surgical implant problems with these specially produced orthopaedic implants are studied, and annual implant engraftment times are studied. Significant progress has been made. The entire 3D x-ray imaging process has been established, including the ability to detect bone edges and display this in 3D, as well as the ability to electronically transfer these files to the rapid prototyping machine. The ability to do segments of skulls as well as hand bones has been demonstrated. The project has produced carpal bones for the hand as well as skull sections using both an organic binder system which was developed, as well as carpal bones using phosphate bonded ceramic materials. What remains to be done are several important steps: (1) determine the mechanical strength properties of the materials being fabricated, (2) establish the actual sizes of the artificial implants produced and establish the shrinkage amounts for the binder-based ceramic implants and allow for this when fabricating the orthopaedic implants, and (3) establish the machining conditions necessary for appropriate surface finish so this process can be controlled. The benefits of this technology are far reaching. First, if the fast setting phosphate-bonded materials show appropriate mechanical strength and body compatibility, then it should be possible to fabricate the implant in the operating room for immediate implantation. Commercialization would seem obvious. What should be commercializable is the fabrication machine, the materials used, and the imaging technology. For the binder-based ceramic materials, even if the time of turn around is 3-6 days, this would allow faster engraftment and thus return to normalcy of the patient. This project directly supports the DOE mission in biotechnology.



**48. Title: High Beam Current, Low Energy Targetry for Production of Radioisotopes for Positron Emission Tomography**

**ID:** BNL95-04

**PI:** David J. Schlyer  
Chemistry Department

**Phone:** 516 344-4587



**Partner:** AccSys Technology, Inc.  
Pleasanton, California

**FY 98 Funding:** \$277K

**Total Project Funds:** \$813K

The major focus of this project is the design of targetry modules which will produce acceptable quantities of a given positron-emitting radioisotope using a windowless or thin window design. These targets will be used on a low energy (7 MeV), high beam current (> 100 microamp) accelerator being marketed by AccSys Technology, Inc. These targets will enable this accelerator to produce useable quantities of radioisotopes for Positron Emission Tomography (PET). The project team's extensive experience in designing cyclotron targets provides a springboard to the development of these new, more demanding targets. A 4 MeV prototype accelerator supplied by AccSys Technology, Inc. is being utilized to carry out the design experiments. The critical tasks which must be accomplished are the design of very thin vacuum isolation windows which will withstand the very high pressures generated inside of the targets, and of very efficient heat removal systems for use with these targets. The high power density of these low energy, high beam current accelerators make heat removal the highest priority. Without these targets, the accelerator can not be used for production of PET isotopes. Therefore, a large potential market is closed to the manufacturer. Although the final target design has not been completed, the accelerator has been operational for approximately one year. However, a series of technical problems with the radio frequency system have prevented full energy tests of the targets. The targets have been designed, built, and are on the beam line awaiting the achievement of full energy. The work carried out in developing these targets has been published in four papers, and abstracts have been presented at four international meetings. This project supports the DOE mission in development of instruments for medical applications.



**49. Title: Methods for Developing Monoclonal Antibodies that Recognize Protein Phosphorylation**

**ID:** BNL98-01

**PI:** Carl W. Anderson  
Biology Department

**Phone:** 516.444-3375



**Partner:** Oncogene Research Products  
Cambridge, Massachusetts

**FY 98 Funding:** \$98K

**Total Project Funds:** \$607K

The project will develop a method that will facilitate making antibodies that recognize any of the many thousands of protein phosphorylation sites in eukaryotic cells with relative ease. The "trick" involves replacing the natural phosphate group with a group that is chemically similar ( $F_2Pab$ ) but that is not recognized by the enzymes in cells that remove phosphates from proteins. This makes the compounds used to immunize animals much more stable; consequently, a much higher fraction of the animal's immune cells produce antibodies that recognize the phosphorylated protein of interest. The method will be tested by developing polyclonal antibodies and monoclonal antibody-producing (hybridoma) cell lines that recognize phosphorylated forms of the human p53 tumor suppressor protein and/or other proteins involved in cell cycle regulation, and the response to DNA damage. If hybridoma producing cell lines are obtained, the project will determine the crystal structure of the antigen-recognizing Fab fragment with the natural phosphorylated peptide and the  $F_2Pab$  derivative. Critical tasks include: (1) identifying a company that can synthesize the t-Boc- or Fmoc- $F_2Pab$  derivative required for preparing peptides, (2) synthesizing normal peptides, chemically phosphorylated peptides, and  $F_2Pab$ -derivative peptides corresponding to several known phosphorylation sites in p53, (3) immunizing rabbits and mice with the derivative compound, and (4) purifying and evaluating the sera and hybridoma cell lines that are produced. Additional tasks involve developing assays that will measure the sensitivity and specificity of each antibody. Approximately one-third of all human cell proteins are phosphoproteins. Thus, the availability of antibodies that recognize single, or groups of phosphorylated sites, should revolutionize molecular studies of eukaryotic cell regulation. The antibodies and assays developed in this project should be of interest to researchers in cell biology, cell cycle regulation, signal transduction, cancer biology, and developmental biology. Oncogene Research Products will explore product formats including development of quantitative assay kits for phosphorylated target proteins. Most importantly, the methods and procedures developed should greatly improve the efficiency of generating the many new reagents that will be required in the future. Finally, novel reagents and methods of detection, based on single-chain antibody constructs, may result from the project. The reagents developed by this project will be of direct benefit to studies designed to understand the consequences of low-dose exposures of human cells to DNA damage producing agents and for functional genomics. These studies are important aspects of DOE's missions to develop fundamental biological information and to advance technologies for use in research on the health effects of energy-related agents and processes.

**50. Title: Biomolecular Contact Lens Material****ID:** LBL94-28**PI:** Carolyn Bertozzi  
Material Sciences Division**Phone:** 510 643-1682**Partner:** Sunsoft Corporation  
Albuquerque, New Mexico**FY 98 Funding:** \$50K**Total Project Funds:** \$510K

Vision is the most important of the human senses, and better ophthalmologic care products are continuously being sought. For example, current synthetic contact lens materials have limited tolerance by the population. The goal of this project is to develop improved materials that will increase the quality of life not only for current wearers but also for those whose physiology cannot tolerate existing materials. In the design of new contact lens materials, the project utilizes the lessons learned in nature. The approach is to modify materials with favorable lens properties so that they more closely resemble biological tissue, and are therefore tolerated well by the eye. The knowledge gained here is expected to further the understanding of how materials behave in a physiological environment and benefit biomedical implant devices development in general. The research represents a significant advance in the development of new biocompatible materials. The first phase in the development of new contact lens materials is the design of biocompatible monomers for incorporation into hydrogel polymers. In order to create lenses that best mimic biological tissue, the project focused on the biomolecules which comprise the coating of most living cells. The strategy is to synthesize polymerizable monomers possessing cell surface-like properties, and to incorporate them into lenses with better biocompatibility characteristics. The project has developed new biological monomers; showed that the composition of their copolymers with poly-HEMA correlates with water content; developed synthetic methods for biomolecular monomers and incorporated them into contact lenses; characterized the bulk and surface properties of the polymers; uncovered an effect of mold composition on surface structure; developed new methods for biomolecular surface coating; and developed a protocol to quantify the adsorption of proteins from a synthetic complex tear solution onto lenses. The interactions of these new materials with corneal epithelial cells will be evaluated in collaboration with researchers at the University of California Berkeley School of Optometry. This project supports DOE's mission in the development of health-related materials research.

**51. Title: Medical Accelerator Technology****ID:** LBL94-36**PI:** William Chu  
Accelerator and Fusion Division**Phone:** 510 486-7735**Partner:** General Atomics (GA)  
San Diego, California**FY 98 Funding:** \$246K**Total Project Funds:** \$1500K

For more than four decades, Lawrence Berkeley National Laboratory has pioneered and developed technologies for treating human cancer using accelerated heavy charged particle (proton and heavier ion) beams, supporting DOE's mission in developing energy technologies for medical applications. In 1991 the first hospital-based medical proton accelerator facility was built in Southern California, and now more than eight hospital-based facilities are being built worldwide by commercial firms. Although the first facility was built by a national laboratory, the subsequent facilities are being built as turn-key systems by the private sector. This project will develop technologies to channel the extracted proton beam from the accelerator to the treatment room, and then deliver it accurately into the treatment volume in a patient. Specifically, the project has developed beam transport systems to bring the protons to the treatment rooms; rotating gantries to aim the treatment beams precisely into patients from any angle; and patient positioners to align the patient accurately relative to the treatment beams. At the Northeast Proton Therapy Center (NPTC) of the Massachusetts General Hospital in Boston, fabrication and installation is almost complete. The accelerator has been installed and successfully tested, and other components are being installed. Commissioning of the facility is scheduled in the fall of 1998. The project is integrating the NPTC medical system for effective therapy delivery providing patient safety. By the end of calendar year 1998, four of the original objectives will be completed. In FY 1999, the project team will design and fabricate the ion source and the low energy beam transport (LEBT) structure. Integrated tests of the ion source and LEBT will be performed. Ion source and accelerator technologies will be transferred to GA for manufacturing of commercial proton therapy tools. Specifically, the project team will design a radio frequency driven multicusp ion source for 13.56 MHz operation with high proton percentage. Computer simulations of ion beam extraction and LEBT systems have been performed. The new LEBT system will conform to the acceptance parameters of the Loma Linda type radio frequency quadrupole (RFQ) injector with the proton beam accelerated to 35 keV. The ion source and LEBT system under development will be versatile and can be applied to different RFQ structures.

**52. Title: A High Throughput Assay for Screening Novel Anti-Cancer Compounds****ID:** LBL98-14**PI:** Mina Bissell  
Life Sciences Division**Phone:** 510 486-4365**Partner:** Genzyme Corporation  
Cambridge, Massachusetts**FY 98 Funding:** \$223K**Total Project Funds:** \$700K

Lawrence Berkeley National Laboratory (LBNL) has pioneered the concept that the micro-environment in which the cell resides, and the cell's surface receptors, are dominant regulators of normal tissue function. They have shown that aberrations in the signals exchanged between the outside and inside of the cell can lead to epithelial cancers such as cancer of the breast and prostate. In a novel model system, LBNL has observed that by manipulating these receptors outside of the tumor, tumor cells revert back to normal. Using a novel tumor cell reversion model based on this observation, the project will develop a high-throughput assay, screen Chiron's library of nearly a million compounds for activity in this assay, and characterize potential lead drugs for novel anti-cancer therapies. The project will screen this assay using combinatorial library technology that will allow the screening of 800,000 compounds in less than two months. This represents a qualitatively different approach to standard molecular target-based cancer drug discovery strategies. Chiron has extensive experience developing high-throughput screening processes, and the bench chemistry scale-up needed to successfully complete this type of project. Chiron also has extensive capabilities in research and development, clinical trials, sales and marketing, manufacturing and other disciplines necessary for success in the health care market. It is one of only a handful of biotech companies that has succeeded in autonomously developing a drug and bringing it to market. This project supports DOE's mission in molecular biology and health applications.

**53. Title: Hydroxylapatite Ontologic Implants****ID:** ORL95-12

**PI:** A. D. McMillan  
Metals and Ceramics Division

**Phone:** 423 241-4554

**Partner:** Smith and Nephew  
Bartlett, Tennessee

**FY 98 Funding:** \$26K

**Total Project Funds:** \$275K

Ontologic implants, because of their small size, are costly to manufacture by the traditional approach of machining from dense hydroxylapatite (HA) ceramic billets. The Oak Ridge National Laboratory (ORNL) gelcasting process has the potential to create these components by net-shape forming these parts. A biocompatible monomer/dispersant system suitable for HA has been developed. Additionally, the project has achieved appropriate green strength, green density, and economical process yields. Green ceramic parts have been both directly cast and green machined and subsequently sintered to full density. The evaluation of the components is almost complete. In this project ORNL has gained a much better understanding of the green machining of soft ceramics, including such parameters as drill speed, bit choice, and depth of cut. The project has also further improved the understanding of the role of surface chemistry in the gelcasting process. Smith and Nephew will decrease their manufacture cycle time and will be able to reduce scrap, thereby cutting their overall cost. This project has demonstrated the application of this technology for producing dense hydroxylapatite components with broad application in biomedical implants. Previously, gelcasting had been licensed to only high-temperature structural ceramic companies. This project supports the DOE missions in advanced ceramics and advanced manufacturing.



**54. Title: The Development of Rhenium-188-Labeled Radioactive Stents for Prevention of Restenosis after Coronary Balloon Angioplasty**

**ID:** ORL98-31

**PI:** F. F. Knapp, Jr.  
Life Sciences Division

**Phone:** 423 574-6225

**Partner:** InnerDyne Inc.  
Sunnyvale, California

**FY 98 Funding:** \$129K

**Total Project Funds:** \$657K

Two approaches for restoring blood flow to the heart are "coronary bypass graft surgery" and "coronary angioplasty," a less expensive clinical procedure, where inflation of a small balloon in the blocked artery restores blood flow. Over 400,000 coronary angioplasties are performed annually in the United States. The reformation of arterial blockage (restenosis) following angioplasty, however, is a major clinical problem since the biological response to this vessel damage is stimulation of accelerated growth of arterial smooth muscle cells. Estimates from the American Heart Association indicate a restenosis incidence as high as 30-40 percent. Therefore, over 120,000 patients per year with coronary restenosis would benefit from methods which would inhibit restenosis of coronary arteries after the angioplasty procedure. The purpose of this project is to develop a new strategy using radioactive stent structures for coronary artery therapy to inhibit restenosis following coronary balloon angioplasty. The use of short-lived radioactive stents is expected to provide a "platform" to keep the vessel open so sufficient radiation to the vessel wall can inhibit restenosis. In addition, this approach will use the same widely used technology for placement of stents by high-pressure balloon expansion. The only difference is that the stent will be radioactive, which requires the institution of radiation protection procedures but does not require new equipment or technical procedures. The objective of this project is the development of fabrication methods which are convenient, economical, routine, capable of being performed in hospitals and other user facilities, and capable of incorporating a choice of radioisotopes such as rhenium-188 which have appropriate dosages required for this application. This project supports DOE's mission of promoting beneficial applications of nuclear technology in human health.



**55. Title: Bioactive and Porous Metal Coatings for Improved Tissue Regeneration**

**ID:** PNL95-23

**PI:** Allison A. Campbell  
Materials and Chemical Sciences Division

**Phone:** 509 375-2180

**Partner:** Implant Innovations Inc.  
Palm Beach Garden, Florida

**FY 98 Funding:** \$60K

**Total Project Funds:** \$597K

The goal of this project is to further develop technologies derived from DOE materials research programs and conduct an experimental program, which, if successful, would provide information necessary to develop a formal manufacturing program for an improved medical device. This project satisfies DOE research interests in fundamental applications of novel materials. Nearly twenty million Americans and more than fifteen million others afflicted with degenerative bone and joint diseases, as well as those who have suffered bone fractures, need devices which anchor to the unaffected bony tissue around the defect site. Although significant advances have been made in the field of metallurgy to provide strong, non-toxic metals and alloys, biological integration of devices into natural tissues remains a problem. Thus, many effective devices become loose over time and necessitate subsequent surgery to replace the old device, a process fraught with high morbidity and mortality. Efforts to solve the problems associated with device anchoring have been highly fragmented among the biological, mechanical, and surgical disciplines. The Surface Induced Mineralization (SIM) process produces a bioactive implant coating/device which may address many of the problems associated with conventional processing methods. The SIM process uses the idea of nature's template-mediated mineralization by chemically modifying the implant to produce a surface which induces heterogeneous nucleation from aqueous solution. SIM produced bioactive coatings provide (1) control of the thickness and density of the mineral phase, (2) a way to coat porous metals, complex shapes and large objects, (3) the ability to coat a wide variety of materials and, (4) a potential choice for the phase of the mineral formed. To date, the project has successfully demonstrated the ability to coat a porous material with bioactive materials. The ability to incorporate biological agents within this bioactive matrix has also been demonstrated. In addition, the project has shown that these coatings signal natural cellular response, in vivo. Currently, almost all synthetic bioactive coatings do not signal the desired biological response.

**Cleaner Industrial Processes****56. Title: Application of Oxygen-Enrichment Technology for Locomotive Diesel Engines****ID:** ANL95-10**PI:** Raj Sekar  
Energy Systems Division**Phone:** 630 252-5101**Partners:** Association of American Railroads  
Pueblo, ColoradoElectro-Motive Division of General Motors  
LaGrange, Illinois**FY 98 Funding:** \$120K**Total Project Funds:** \$830K

Railroad operators and locomotive diesel engine manufacturers are facing a major challenge meeting the EPA's proposed emissions standards for in-use and future locomotives. On the basis of the date (from 1973 through 2005 and later) that a locomotive is first manufactured, three separate sets of standards are proposed. Railroads also face an increasing demand for higher motive power because of recent developments in a/c traction, so payloads in freight locomotives (revenue) can be increased. The goal of this project is to apply the oxygen-enriched combustion technology for locomotive diesel engines to achieve low emission levels. Because of the increased oxygen content, combustion is more complete resulting in lower particulates, visible smoke, and unburned hydrocarbons. Additional fuel can be burned effectively resulting in an increase in power output. The reduction in ignition delay period with oxygen-enrichment provides an opportunity to control NO<sub>x</sub> emissions by retarding the injection timing. This will enable the railroads and engine manufacturers to meet the goals of lower exhaust emissions and higher motive power from locomotives in a cost-effective manner. This project has conducted laboratory engine tests on a two-cylinder locomotive research engine to obtain the performance and emissions data at different levels of oxygen-enriched air by using an external oxygen source. The test results show that with the optimized oxygen-enrichment level in the intake air, fueling rate, and injection timing, both particulates (lower by 60-80%) and NO<sub>x</sub> (lower by 10-25%) emissions can be reduced simultaneously. In addition, higher gross power by 15-30% can be achieved with minimal increase in peak cylinder combustion pressure. In order to reduce NO<sub>x</sub>



emissions further, engine tests are currently underway with a lean NO<sub>x</sub> catalyst in collaboration with a diesel catalyst manufacturer. The project has developed appropriate bench test facilities to characterize the air separation membrane for locomotive diesel engine applications. The next step in the project is to demonstrate the technology on a research engine (two-cylinder EMD 567B) in the laboratory, while using an air separation membrane supplying the desired oxygen-enriched air in the engine intake and with a lean NO<sub>x</sub> catalyst in the exhaust controlling NO<sub>x</sub> emissions. The project supports DOE's mission in improving the efficiency, economic competitiveness, and future environmental compliance of the railroad industry. The successful demonstration of the technologies in this project will assist the railroad industry in producing more power locomotive diesel engines without a costly R&D program, assist in meeting the EPA's emissions standards, and improve the international competitiveness of U.S. locomotive manufacturers.

**57. Title: Nonconsumable Metal Anodes for Primary Magnesium Production**

**ID:** ANL98-05

**PI:** Michael J. Pellin  
Materials Science/Chemistry Divisions

**Phone:** 630 252-3510

**Partner:** Dow Chemical Company  
Freeport, Texas

**FY 98 Funding:** \$210K

**Total Project Funds:** \$750K

This project will develop a nonconsumable metal anode to replace consumable carbon anodes now used in commercial electrolysis cells for primary magnesium production. The use and manufacture of consumable carbon anodes, which must be constantly replaced, is costly, energy consuming, and occasions unwanted gaseous emissions such as CO<sub>2</sub> and HCl. In support of the DOE mission for energy efficient, environmentally sound industrial processes, ANL has identified certain metal alloys that are promising candidate materials for nonconsumable anodes. Such alloys form self-limiting surface oxide films that are thin enough to allow current to pass, yet thick enough to prevent attack of the underlying metal. These alloys are dynamic in that the more volatile, reactive components segregate to the surface at rates sufficient to reform the

protective film as it dissolves in the chloride melt. The project will form surface films on candidate alloys and investigate them using surface analysis instruments and techniques. Promising alloys will be tested as anodes in bench-scale magnesium electrolysis cells. Cell operation will be monitored and interrupted at key points to remove the anode and investigate its surface film. If desirable, the anode film thickness and strain during electrolysis in specially designed cells will be studied. Alloys identified as optimal will be subject to long-term bench-scale tests by Dow Chemical Company, and then tested in full-scale cells at Dow's production facility in Freeport, Texas. Successful completion of this work will result in increased U.S. competitiveness and lower magnesium prices which would, for example, allow magnesium to be used more widely in the transportation sector, resulting in lower costs there. If successful, stable anodes would reduce the operating cost of making magnesium by 20-30 % and eliminate the emission of CO<sub>2</sub> and other halocarbon gases during magnesium production by eliminating the need for carbon anodes, now used to produce magnesium electrolytically. Moreover, this work will illuminate the mechanisms associated with film formation on alloys. An understanding of these mechanisms (e.g., surface segregation, near surface diffusion) will provide the basis for developing a new class of corrosion resistant materials that can find application in harsh chemical environments, for example as nonconsumable anodes for aluminum production.



**58. Title: Advanced Separations Technology for Efficient and Economical Recovery and Purification of Hydrogen Peroxide**

**ID:** ANL98-07

**PI:** Edward J. St. Martin  
Energy Systems Division

**Phone:** 630 252-5784

**Partners:** Unitel Technologies, Inc.  
Mt. Prospect, Illinois

UOP  
DesPlaines, Illinois

**FY 98 Funding:** \$125K

**Total Project Funds:** \$750K

Hydrogen peroxide is an effective oxidant that could be used in many industrial processes. However, the current method for production is inefficient and too costly. Because the only byproduct of oxidation using hydrogen peroxide is water, it could become the ultimate green chemical for the manufacture of oxygenated petrochemicals. The objective of this project is to develop an efficient, economical and safe process for the manufacture of hydrogen peroxide that utilizes advanced membrane separations technology with improved catalysts and processing technology. Argonne National Laboratory will develop an economical separations process for aqueous hydrogen peroxide from organic hydrocarbon containing reaction mixtures based upon pervaporation membrane technology. UOP will provide proprietary hydrogenation catalysts that confer higher specificity and lower losses. Unitel Technologies will provide improved organic formulations and process development. The combination of these three developments in the new hydrogen peroxide process represents a radical departure that promises to significantly change the way hydrogen peroxide is made and used. Not only could this be a simpler, more benign, and less expensive process, but it would also allow the development of new commercial applications and markets for hydrogen peroxide that are currently not competitive. In addition, it could allow small-scale systems to be built on site thus enabling rapid increases in capacity and point of use plants. This project supports the DOE mission in advanced environmental technologies that use advanced membrane technologies for solving fundamental issues in chemical processing and pollution prevention.



**59. Title: Condensing Economizers for Improved Efficiency and Reduced Pollution**

**ID:** BNL94-22

**PI:** Thomas Butcher  
Department of Applied Science

**Phone:** 516 344-7916

**Partners:** Babcock and Wilcox  
Barberton, Ohio

Consolidated Edison Company of New York, Inc.  
New York, New York

**FY 98 Funding:** \$159K

**Total Project Funds: \$825K**

Condensing economizers recover sensible and latent heat from boiler flue gas, leading to marked improvements in thermal efficiency. These economizers, in addition, have the potential to serve as pollution control devices, capturing SO<sub>2</sub>, particulates, and air toxics. Configured for pollution control, these systems have been named Integrated Flue Gas Treatment (IFGT) systems. The main objective of this project is to develop IFGT technology so that it will be strongly attractive commercially, providing a viable method of both improving energy efficiency and reducing pollutant emissions from boilers. Expected new products resulting from this work include a variety of IFGT systems. These will reduce operating costs of power generation and process plants through increased energy efficiency. In addition, these will offer attractive options for sites that need to reduce particulate, air toxics, and SO<sub>x</sub> emissions. The target market includes existing gas, oil, coal, wood, and waste-fired plants ranging in size from light industrial to utility. At Brookhaven National Laboratory (BNL) small-scale pilot research is being done with an emphasis on mechanisms of particulate capture. Several methods of enhancing particulate capture have been investigated. For particles over 1 micron, high removal efficiencies have been achieved. Overall, for oil firing, removal efficiencies of 90-95% have been achieved. In current work, BNL is looking at the condensation of acid aerosols, submicron particulate removals, and effects of operating conditions. Babcock and Wilcox is doing larger scale, application specific pilot tests with an emphasis on SO<sub>2</sub> and air toxics capture. The flue gas pollutants being studied include ammonia, hydrogen chloride, hydrogen fluoride, gas phase and particle phase mercury, and gas phase and particle phase trace elements. At Con Edison, a full scale, 30 MW demonstration/test program is in progress. This project supports DOE's mission in improving environmental quality.



**60. Title: Catalytic Production of Organic Chemicals Based on New Homogeneously Catalyzed Ionic Hydrogenation Technology**

**ID:** BNL97-05

**PI:** R. Morris Bullock  
Chemistry Department

**Phone:** 516 344-4315

**Partner:** DuPont Company  
Wilmington, Delaware

**FY 98 Funding:** \$235K

**Total Project Funds:** \$705K

Homogeneous transition metal-catalyzed hydrogenations are practiced widely in the chemical industry to synthesize products ranging from high-volume commodity chemicals to small-scale, high-value pharmaceutical products. Improvements in activity and selectivity are ongoing challenges for the chemical industry. The purpose of this project is to develop new technology for the catalytic production of organic chemicals of commercial interest. The scientific objectives are to explore the feasibility, scope, and selectivity of catalytic ionic hydrogenation technology, in which hydrogen is added to an organic chemical in the form of a proton followed by a hydride. DuPont uses catalytic ketone hydrogenations in the synthesis of their agricultural and pharmaceutical products. Many industrial catalytic processes utilize expensive precious metals such as rhodium. A series of new catalysts based on the inexpensive and abundant metals molybdenum and tungsten were recently examined in the project. These molybdenum and tungsten catalysts carry out catalytic ketone hydrogenations under remarkably mild conditions: room temperature and low pressures of hydrogen gas. A detailed evaluation of these catalytic reactions is underway, including an evaluation of the effect of variation of steric and electronic properties of phosphine ligands bonded to the metal catalyst. Identification of the mechanism of catalyst deactivation will provide guidance for the design of more efficient and longer-lived catalysts. Ionic hydrogenations also present the possibility of carrying out new selective transformations unattainable with traditional hydrogenation catalysts, such as the selective reductive dehydroxylation of polyols for the conversion of biomass-derived materials to fine chemicals as well as basic feedstocks. DuPont is also interested in using selective catalytic reductive dehydroxylation to convert polyols into diols, for use as polymer intermediates. These reactions may lead to useful commercial processes and are also attractive for environmental reasons, as they employ alternative renewable feedstocks rather than petroleum-based feedstocks. A ruthenium catalyst system that accomplishes the catalytic dehydroxylation of diols has been developed. Hydrogen pressure, temperature, and other reaction parameters are being systematically varied in order to optimize this reaction and develop a molecular-level understanding of the mechanism. This project supports DOE's mission of obtaining an improved molecular understanding of the mechanisms of catalytic chemical reactions as well as the development of new means of conversion of biomass materials to useful chemicals.

**61. Title: Catalytic Conversion of Chlorofluorocarbons over Palladium-Carbon Catalysts****ID:** LBL95-45**PI:** Gabor A. Somorjai  
Materials Sciences Division**Phone:** 510 486-4831**Partner:** DuPont Company  
Wilmington, Delaware**FY 98 Funding:** \$30K**Total Project Funds:** \$257K

Chlorofluorocarbons must be replaced by fluorocarbons as refrigerants and chemicals because of their adverse health effects (ozone depletion and other effects). The hydrodechlorination of  $C_2F_4Cl_2$  to  $C_2F_4H_2$  using palladium catalysts supported on carbon achieves this goal. This project investigates the kinetics and mechanism of this reaction using palladium foils and single crystals as catalysts. From reaction rate studies, the kinetic parameters for the reaction have been determined along with many of the elementary reaction steps. The structure and bonding of reactants and products on various single-crystal palladium surfaces have also been determined. The causes for catalyst deactivation have been studied along with the roles of the carbon support to influence catalytic reaction rate and selectivity. The desired  $C_2F_4H_2$  molecules are formed in parallel with other competing reaction products and the inhibition of these side products was investigated. The adsorption of the molecular  $C_2F_4Cl_2$  reactant is the rate-determining step for the process. The reaction is surface structure insensitive; sulfur causes deactivation, and the carbon support plays a minimal role during the catalytic reaction. Early results indicate that hydrogenation of chlorofluorocarbons with solid state hydrogen is much more selective and occurs at a higher rate than hydrogenation using gaseous hydrogen. The project is exploring the palladium-catalyzed hydrodechlorination of chlorofluorocarbons to produce fluorinated olefins. These are important reaction intermediates that can be used to produce new fluorocarbons in addition to tetrafluoroethane. The project will study the hydrogenation ability of solid state hydrogen that is stored in the bulk palladium. This project supports DOE's mission in environmental quality and advanced materials processing.

**62. Title: Moving an Advanced Desiccant Material into Mainstream non-CFC Cooling Products****ID:** ORL95-06**PI:** Phillip D. Fairchild  
Energy Division**Phone:** 423 574-2020**Partner:** Engelhard/ICC  
Philadelphia, PA**FY 98 Funding:** \$50K**Total Project Funds:** \$640K

This project focuses on advancing desiccant-based systems for cooling buildings. The goal is to develop the enabling technologies that will foster the acceptance of desiccant-based equipment into the mainstream of the U.S. commercial air-conditioning market. Barriers to the broad acceptance of desiccant technology are: (1) a perception of inefficiency from earlier research on desiccant space-conditioning systems; (2) lack of suitable metrics to evaluate desiccant-based system performance against conventional systems; and (3) absence of computerized algorithms that allow conventional incorporation of desiccant modules in heating, ventilation, and air conditioning (HVAC) simulation programs used by evaluation and application engineers. The critical tasks to be accomplished include (1) identifying two target HVAC applications for desiccant-based products; (2) developing computerized desiccant-component performance-evaluation and system-simulation tools for building-specification design engineers and architects; (3) preparing a draft performance-evaluation methodology, product rating, and system comparison standard for the desiccant air-conditioning industry; and (4) completing a cost/performance versus market penetration analysis for desiccant products. Desiccant systems can potentially reduce building energy consumption, decrease emissions of greenhouse gases, reduce the use of halogenated refrigerants, reduce electrical peak demand, improve indoor air quality and comfort control, and create jobs in the manufacturing and service sectors in support of DOE missions. To date, a 2,600 cubic feet/ minute desiccant system has been installed in the laboratory for testing over a range of different ambient conditions. Instrumentation, including humidity sensors, gas and water-flow meters, differential pressure transducers, air-flow meters, and temperature sensors, is being installed to determine the performance of the system, while varying operating parameters such as wheel speed, air flow rate, and desiccant material.

**63. Title: An Air Conditioning System with Improved Efficiency for Hybrid/Electric Vehicles****ID:** ORL95-09**PI:** Donald J. Adams  
Engineering Technology Division**Phone:** 423 576-0260**Partners:** Nartron Corporation  
Reed City, MichiganAdvanced Vehicle Systems, Inc.  
Chattanooga, TennesseeChattanooga Area Regional Transit Authority  
Chattanooga, TennesseeElectric Transit Vehicle Institute  
Chattanooga, Tennessee**FY 98 Funding:** \$70K**Total Project Funds:** \$670K

The primary technical goal of this project is to develop an advanced, highly efficient electric motor and controller for a mobile air conditioning compressor for an electric bus air conditioner system. The objective is to improve the air conditioner system efficiency so that the useful bus range is extended. This project supports DOE's mission in electric and hybrid electric vehicle development. To achieve this goal, the efficiency of the Nartron Corporation's technically advanced, high efficiency, microprocessor controlled, turbine driven, modular air conditioner will be further improved. The mass and size of the compressor motor will be reduced by incorporating advanced electric machinery systems technology that is only available at Oak Ridge National Laboratory (ORNL). The advanced system will then be installed in an Advanced Vehicle Systems (AVS) electric bus that will be operated by the Chattanooga Area Regional Transportation Authority (CARTA) with Electric Transit Vehicle Institute liaison. An air conditioning system with existing motor technology will be run on the same bus for comparison. The electrical and mechanical design of an axial gap permanent magnet motor with challenging size and power constraints has been completed. The first prototype hardware including housing and assembly fixtures is nearly complete. ORNL has completed the stators and windings, but



Nartron has had considerable difficulty in obtaining the novel rotor and shaft sub-assembly from the supplier. The rotor and shaft assembly was recently received at Nartron, but the ring magnet broke during re-assembly into the housing, due to a known fault in the magnet. A new rotor was expected from the supplier in July 1998. Assembly will then proceed, followed by testing and evaluation prior to installation in a bus. A self-sensing controller and power inverter for the permanent magnet machine has been completed at ORNL. Nartron had considerable difficulty in procuring a suitable alternate technology radial gap motor, but finally did succeed in delivering such a system to AVS. Continuing development and a revised compressor design have heightened the importance of ORNL's contribution to the project. All simulations have predicted much improved efficiencies for both the motor and controller, and the reliability should be much improved.

**64. Title: New Thermoelectric Materials**

**ID:** ORL95-10

**PI:** Brian C. Sales  
Solid State Division

**Phone:** 423 576-7646

**Partner:** Marlow Industries  
Dallas, Texas

**FY 98 Funding:** \$85K

**Total Project Funds:** \$700K

The goal of this project is to develop materials that will improve the performance of thermoelectric devices for solid state refrigeration and power generation. Thermoelectric devices have no moving parts, use no greenhouse gases, and are extremely reliable. The poor efficiency of commercial thermoelectric devices, however, has restricted their use to applications in which reliability or convenience are more important than economy. In support of the DOE missions for energy efficient technologies and basic materials programs, ORNL has evaluated several classes of compounds as possible advanced thermoelectric materials, including materials with the filled skutterudite crystal structure, and unusual "Kondo-like" metals and semiconductors. Marlow Industries has participated in the materials selection process, has provided guidance on thermoelectric materials and concepts, and will fabricate thermoelectric refrigeration devices for a more complete evaluation of promising materials. Based on the

current experimental data, the most promising approach is to design ternary semiconductors in which one of the atom types is weakly bound in an oversized atomic cage. The "rattling" motion of the caged atom can dramatically lower the ability of the solid to conduct heat. Good electrical conduction is maintained through the atoms comprising the cage. The project has demonstrated that for the filled skutterudite antimonides, this approach results in materials with thermoelectric efficiencies at elevated temperatures (700-1000K) that are as good or better than all previously studied materials. Current efforts are aimed at using this same approach to create improved thermoelectric materials that operate at the below room temperature.



**65. Title: Development of Tape Calendaring Technology for Separation Membranes**

**ID:** PNL95-04

**PI:** Timothy Armstrong  
Materials and Chemical Sciences Division

**Phone:** 509 375-3938

**Partner:** Air Products  
Allentown, Pennsylvania

**FY 98 Funding:** \$370K

**Total Project Funds:** \$750K

The purpose of this project is to develop tape calendaring technology to produce passive oxygen separation membranes from mixed conducting ceramics, and to transfer that technology to Air Products. Successful development of passive oxygen separation membranes will support DOE missions for energy efficient industrial processes in two ways by: (1) directly reducing the amount of energy used in producing purified oxygen, and (2) indirectly reducing the energy used in other industrial processes, as a result of reducing the cost for purified oxygen that may be used in these processes. In order to successfully develop these membranes, methods are needed to produce membrane structures that balance high flux requirements and robust mechanical properties. Tape calendaring combines oxide powders, binder, and plasticizer in a high-intensity mixer. The binder-plasticizer system can be softened by externally heating the mixing chamber, using only internal heating resulting from frictional forces generated within the mixing chamber, or combinations of the two. The softened binder system mixes with the ceramic powder to form

a plastic-like mass. The mass is calendered into a thin, flat tape using a two-roll mill with counter rotating rolls. Tape thickness is controlled by the spacing of the two rolls. Tape calendering technology shows exceptional promise as a means to manufacture complex ceramic structures on a large scale and at low cost. If successful, this project could provide key technology that would help Air Products produce large quantities of oxygen at a significantly lower cost (40-50%) than current cryogenic methods. This project has resulted in a method to manufacture both monolithic (self-supporting) and asymmetric (thin-film on a porous support) membranes using tape calendering. Several different material compositions provided by Air Products have been fabricated into membranes and delivered for testing. In addition, the process has been scaled up from laboratory scale to a size comparable to a small prototype line. Scale up has resulted in small production runs of several square feet to tens of square feet. These tapes have been delivered for testing. The asymmetric membranes produced by this method show high oxygen flux rates consistent with theoretical predictions, significantly higher than membranes made by other fabrication methods. The high flux rates are due to the reduction in thickness of the dense gas separating membrane. This fabrication method is inexpensive, costing approximately \$15/square meter of material and is comparable to tape cast materials (\$19/square meter).

**66. Title: Solid Acid Environmental Catalysis****ID:** PNL95-27**PI:** John Nicholas  
Environmental and Molecular Sciences Division**Phone:** 509 375-6559**Partner:** Catalytica, Inc.  
Mountain View, California**FY 98 Funding:** \$83K**Total Project Funds:** \$291K

The purpose of this project is to develop new catalytic materials and processes that have little or no impact on the environment. Most industrial catalytic processes involve toxic liquid acids and bases, which are dangerous to work with and difficult to dispose of. Another objective of

the project is to understand the atomic-level details of catalysis, with the eventual goal of developing new catalysts that are environmentally benign. Pacific Northwest National Laboratory (PNNL) will develop theoretical predictions about the function of the new catalysts, which will be complemented by experimental evaluation and verification by Catalytica. In this way, the unique computational capabilities of the Environmental and Molecular Sciences Laboratory will be used to elucidate the fundamental aspects of catalysis, which are needed in order to support the DOE mission to develop new environmentally-benign products. Whereas many large-scale processes used in the petroleum and chemicals industries rely heavily on catalysis, the development of a new catalytic process could have a significant effect on the U.S. economy. In addition, catalytic processes that reduce energy consumption, or lead to alternative fuel sources, could greatly reduce U.S. dependence on foreign oil supplies, supporting the DOE mission for energy security. The project is studying the mechanisms of two new catalysts developed by Catalytica. These catalysts convert methane, which commonly must be burned at remote oil drilling sites, to methanol, a liquid that can be safely transported and processed into an alternative energy source. The theoretical investigations have all been done using quantum mechanical methods, primarily high level ab initio molecular orbital techniques. The project investigated the reaction mechanism for the conversion of methane to methanol, using a Hg catalyst in  $\text{H}_2\text{SO}_4$  solvent. The project also studied how the use of other metals (Cd and Zn) and other solvents ( $\text{CF}_3\text{SO}_3\text{H}$  and  $\text{CF}_3\text{CO}_2\text{H}$ ) affects the reaction barriers. The project also focused on the validation of new theoretical methods that can be applied to catalyst design. The model systems needed in order to obtain an accurate picture of the catalytic system are often large, and calculations on them require extensive computational resources. The NWChem computer code recently developed by PNNL for massively parallel computers is being evaluated for catalyst research.



**67. Title: Highly Dispersed Solid Acid Catalysts on Mesoporous Silica**

**ID:** PNL97-28

**PI:** Yong Wang  
Chemistry Division

**Phone:** 509 376-5117

**Partner:** UOP Research Center  
Des Plaines, Illinois

**FY 98 Funding: \$250K**

**Total Project Funding: \$750K**

Homogeneous acid catalysts such as sulfuric acid and aluminum chloride are currently used to catalyze many industrially important reactions. Although these homogeneous acid catalysts are efficient, they are not environmentally benign and create many operational problems. These problems can be mitigated with solid acid catalysts. Tungstophosphoric acid and sulfated zirconia are two solid acid catalysts with super acidity, yet both suffer from low catalytic efficiency. In addition, it is difficult to disperse tungstophosphoric acid on supports due to its large cluster size, and sulfated zirconia generally suffers rapid deactivation. These problems can be minimized with the superior characteristics of mesoporous silica. This project aims to develop new materials optimized for use as solid acid catalysts by coupling the advanced characteristics of mesoporous silica with the superacidic properties of tungstophosphoric acid and sulfated zirconia. The goal is to exceed the performance characteristics of existing solid superacid catalysts, thereby enabling the chemical and petrochemical industries to replace homogeneous acid catalysts. This will contribute to DOE's mission to reduce environmental impacts in the energy sector. This project has functionalized the surface of mesoporous silica for the dispersion of tungstophosphoric acid and sulfated zirconia acid groups. Novel methods to graft tungstophosphoric acid using  $\text{Cs}_2\text{CO}_3$  as the anchoring agent, and to graft hydrous zirconia via in-situ hydrolysis have been developed. Highly dispersed solid acid catalysts with controlled loading density have been synthesized and characterized. The novel catalysts have been tested with two model reactions in the bench-scale testing unit, i.e., alkylation of mesitylene by cyclohexene and n-butane isomerization. The activity testing results indicate that monolayer sulfated zirconia on mesoporous silica may not possess the superacidity as that of bulk sulfated zirconia, and highly dispersed Cs-tungstophosphoric acid salt is not active as desired. Thorough characterization and further improvement in synthesis are being performed in order to understand the physical and chemical properties of highly dispersed solid acid catalysts, and to optimize their catalytic performance.

Environmental Technologies**68. Title: A Pilot Scale Demonstration of Citric Acid Technology****ID:** BNL95-13**PI:** A.J. Francis  
Department of Applied Science**Phone:** 516 282-4534**Partner:** Forrester Environmental Services, Inc.  
Hampton, New Hampshire**FY 98 Funding:** \$77K**Total Project Funds:** \$438K

The objective of this project is to remove toxic metals such as lead and cadmium from incinerator ash using the Citric Acid Process developed at Brookhaven National Laboratory. In this process, toxic metals in bottom ash from the incineration of municipal solid waste were first extracted with citric acid followed by biodegradation of the citric acid-metal extract by *Pseudomonas fluorescence* for metals recovery. The ash contained the following metals: Al, Ba, Ca, Cd, Cr, Cu, Mg, Mn, Ni, Pb, and Zn. The extraction efficiency of lead by citric acid was affected by its mineralogical association in the ash. Optimization of the citric acid process, which included the effects of citric acid concentration, contact time, the impact of mixing aggressiveness during extraction, and pretreatment of ash, resulted in the removal of >97% of lead from incinerator ash allowing to pass the Toxicity Characteristic Leachability Procedure. Biodegradation of citric acid extract removed >99% of the lead from the extract as well as other metals such as Al, Ca, Cu, Fe, Mg, Mn, Ti, and Zn. Speciation of lead associated with the biomass, after biodegradation of citric acid extract by x-ray absorption spectroscopy techniques at the National Synchrotron Light Source, showed that the precipitated lead is predominantly associated with the phosphate and carboxyl groups. After the solubilized metals were removed using a sulfide precipitation technique, the citric acid was completely recovered (>99% yield). The recycled citric acid proved as efficient an extractant as fresh material. These results suggest the potential application of this technology to remove and recover the metal contaminants from incinerator ash and from other waste forms. Information developed from this project is being applied to remediate Pb paint bearing soils and the removal of Pb and other toxic metals from electric arc furnace (EAF) dust from the steel industry. This project supports DOE's mission in environmental quality and pollution prevention.

**69. Title: Vehicle Exhaust Treatment Using Electrical Discharge and Materials Chemistry****ID:** PNL95-10**PI:** Thomas Orlando  
Environmental and Molecular Sciences Division**Phone:** 509 376-2847**Partner:** USCAR  
Dearborn, Michigan**FY 98 Funding:** \$120K**Total Project Funds:** \$750K

This project will help determine the feasibility of using non-thermal plasmas in conjunction with catalytic materials to mediate exhaust gas emissions from an internal combustion engine, which directly supports DOE's mission for an efficient low emission vehicle. The project is directed toward developing an understanding of plasma activated processes which can be exploited to reduce NO<sub>x</sub> emissions under lean burn (highly oxidative) conditions. Work is focused on the plasma and materials issues that will ultimately allow the development of a device for reductive elimination of NO<sub>x</sub> from lean burn exhaust streams. The device should also simultaneously oxidize hydrocarbons while reducing NO<sub>x</sub>. Technologies will be evaluated with a goal of supplementing or replacing existing automobile catalytic converters. This work is also being evaluated with respect to its applicability to compression ignition (diesel) emissions. A systematic study has been done of the destruction of low concentrations (<600 ppm) of NO and NO<sub>x</sub> in synthetic lean-burn exhaust mixtures using a two-stage reactor. The two-stage reactor utilizes a dielectric barrier corona discharge in the first stage and a thermally activated catalyst in the second. Using this reactor, the project has achieved up to 65% overall NO<sub>x</sub> removal at relatively modest input energies (e.g. 3.4% of the input fuel). The two stage reactor allows separation of the discharge chemistry from the surface chemistry. Analysis of the data indicates that the plasma chemistry is required for oxidation of the NO as well as partial oxidation of hydrocarbons in the exhaust stream. The second stage allowed rapid screening of candidate catalysts under identical plasma conditions. Variation of the background gases in the synthetic exhaust in conjunction with gas chromatography allowed the quantification of N<sub>2</sub> production during NO<sub>x</sub> treatment. Direct detection of N<sub>2</sub> from non-thermal plasma processing of NO<sub>x</sub> had not been previously demonstrated due to high concentrations of N<sub>2</sub> in exhaust. However, the project demonstrated that 88% of the NO<sub>x</sub> lost appeared as nitrogen product. These results provide a strong indication of the potential for non-thermal plasmas (in conjunction with

appropriate catalytic materials) to provide a means for the elimination of NO<sub>x</sub> (and possibly other) emissions from lean burn vehicle exhaust streams. Due to these promising results, USCAR has substantially increased its resource commitments to the project. This increased commitment has been matched by an increase in funding from the Office of Transportation Technologies.



**MAJOR INDUSTRY PARTNERSHIPS****Advanced Computational Technology Initiative (ACTI)****70. Title: Development of a New Generation Framework for Parallel Reservoir Simulation****ID:** ANL-ACTI-95-95**PI's:** Tom Morgan  
Mathematics and Computer Science Division**Phone:** 630 252-5218**Partners:** ARCO, BP Exploration, Chevron, Conoco, Cray Research, IBM, Landmark Graphics, Mobil, Scientific Software-Intercomp, Schlumberger-GeoQuest, Texaco, Unocal**FY98 Funding:** \$219K**Total Project Funds:** \$969K

The simulation of petroleum reservoirs is an important component in the development of more efficient techniques in oil recovery. Current simulators used routinely in industry are fundamentally limited in the size and complexity of the problems they can handle. Only through the use of parallel computing will the industry be able to tackle problems of current interest. This project provides much underlying research and development (the physics, mathematics, and computer science) for the next generation of simulator codes. The results of this project also closely relate and apply to the simulation, and therefore understanding, of underground pollution plumes and other subsurface phenomena requiring site characterization, supporting DOE's mission in environmental management. An important milestone was recently reached. The project has run a series of parallel 3D reservoir simulations using the compositional simulator. The largest test so far involved four million gridblocks and 32 million unknowns and took approximately 23 minutes to run on a 128-processor IBM SP. This may be one of the largest and fastest compositional reservoir simulations made to date, and illustrates the potential of efficient parallel computing. The focus of this development has been to increase the speed of the simulations to the point that almost all of the description data can be used directly. High-end compositional simulations are of special interest to large-scale improved oil recovery projects, such as the solvent injection effort for the mammoth Prudhoe Bay oil reservoir. This supports DOE's mission in managing the strategic petroleum reserve. Further testing for scalability and portability to other environments is underway. Industry does not typically do the kind of research around which this project is structured. However, the advancement of industry reservoir simulators is likely to be critically dependent on many elements of this research. This work offers a basis for new

parallel simulators by oil and environmental companies and commercial software vendors. Key features include the ability to run realistic, high-resolution reservoir/aquifer studies; to model realistically complex physical processes including compositional, chemical, geochemical; and to perform conditional simulations efficiently and rapidly. When resultant research elements are ready for application, the industry participants, whether petroleum companies or service companies, should be able to employ/adapt this work into their own proprietary simulators.

**71. Title: Subsalt Imaging with Marine Magnetotellurics****ID:** LBL-ACTI-95-90**PI:** H. Frank Morrison  
Earth Sciences Division**Phone:** 510 486-5080**Partners:** Amoco, BP, Chevron, Exxon, Geotools Corporation, NWG Associates, Texaco, Unocal, Conoco**FY 98 Funding:** \$90K**Total Project Funds:** \$1050K

Marine magnetotellurics (MT) is a new technique to augment seismic imaging in geological surveys. MT can reveal the size and thickness of underwater salt structures using differences in natural electromagnetic radiation in rock structures. This information can help researchers gauge the prospects for the sediment underlying the salt to be rich in oil or gas. Lawrence Berkeley National Laboratory (LBNL) is specifically assisting the industry partners in the development of software algorithms and computer simulation models used in the analysis of the MT data. Scientists at LBNL are initially developing inversion code for the two dimensional computer depiction of MT field data. In follow-on tasks, LBNL will extend the code development to integrate seismic, gravity, and MT data for two and three dimensional depictions of survey areas. Initial work is on potential oil and gas fields in the Gulf of Mexico. A series of numerical simulations of 2D and 3D salt structures has shown that MT should be able to map the base of salt structures. For field testing, a hardware package to acquire MT data from the sea floor was developed at Scripps, and data processing software was developed at LBNL and University of California at Berkeley. Initial field surveys have

been conducted at two sites in the Gulf of Mexico. The first survey, conducted in August 1996 went well but the data were too noisy to be useful. The second survey, conducted in July 1997 after instrument problems were corrected, went extremely well, providing impressive imaging of salt shapes using new numerical codes developed for the project. Oil exploration companies are very interested in commercializing the results of this project. This project supports the DOE mission in energy security.



**72. Title: Optimal Fluid Injection Policy and Producibility in Fractured, Low Permeability Reservoirs**

**ID:** LBL-ACTI 95-92

**PI:** Tad Patzek  
Earth Sciences Division

**Phone:** 510 643-5834

**Partner:** Aera Energy  
Bakersfield, California

**FY 98 Funding:** \$87K

**Total Project Funds:** \$750K

In low-permeability oil reservoirs (diatomites, chalks, and carbonates), primary production yields only 2% to 6% of the oil-in-place. Fluids such as water, steam, or carbon dioxide are injected into these reservoirs to increase or sustain oil production and prevent reservoir damage. An optimal injection policy minimizes formation damage while maximizing oil production per unit volume of injectant. The purpose of this project is to provide the oil industry with tools to optimize injection policies in the low-permeability reservoirs. Fluid injection into low-permeability reservoirs either for pressure maintenance or secondary oil recovery is very difficult. This project is developing an innovative set of Computer-Assisted-Operations tools to promote higher and cheaper recovery from fractured, low-permeability diatomite fields in Kern County, California. The tools function by making optimal, or "expert," decisions that balance fluid injection rate and fluid injection pressure goals versus the capacity of the reservoir to sustain hydrofracture extension and formation damage, with the subsequent decrease of oil production, injectant recirculation, and well failure. Features of this project include: (1) real-time, well-by-well passive monitoring of injectors and their associated

fractures, and the progress of injected fluid; (2) software tools to compile and evaluate the injector performance; (3) active monitoring of hydrofracture growth and well coupling; and (4) optimal model-based wellhead controllers of fluid injection. The project has demonstrated that neural networks are capable of predicting injection rate as a function of wellhead injection pressure and vice-versa. The first generation of neural network controllers has been developed and deployed on Aera Energy's server. The project has also observed that neural network predictions and, therefore, neural network controllers, may become unstable if the injector dynamics changes sufficiently. To quantify better the injector dynamics, the project has developed a software package, I.D.E.A. (Interactive Data Evaluation and Analysis Tool). The project has found that at constant injection pressure the injection rate is remarkably constant. The project has shown that pressure control may be stable, but rate control is not. A semi-continuous measurement of wellbore and hydrofracture acoustics may be required to update the controller parameters. The project has constructed, and is evaluating for possible patent, an optimal controller to stabilize the injection rate near a prescribed value. Recently, several features were added to the Interactive Waterflood Analyzer allowing interactive exploration of the production data from an oil field, either on a well-by-well basis or on a multiple-well basis. The program allows assessing the waterflood response of the wells, and also performs a comparative evaluation of the performance of any given well and its natural neighbors.



**73. Title: Advanced Computational Analysis of Drill Cuttings for Real-Time Well Site Decisions**

**ID:** LBL-ACTI-95-94

**PI:** Larry R. Myer  
Earth Sciences Division

**Phone:** 510 486-6456

**Partners:** BP-America  
ARCO, E&P Technology  
Houston, Texas

Meridian Oil, Inc.  
Houston, Texas

**FY 98 Funding:** \$190K

**Total Project Funds: \$2955K**

Today the engineer on a drill rig platform possesses limited information about the properties of the subsurface being drilled thousands of feet below. Nonetheless, critical decisions must be made "on-the-spot" with regard to the stability of the well and the location and quality of reservoir rock. This project focuses on development of a new technology utilizing rock fragments produced during drilling to provide the information on rock properties needed to make these rig-site decisions. The successful implementation of this technology is estimated to yield at least 300 million barrels of oil equivalent, as bypassed producing zones are developed, and missed opportunities are reduced, supporting DOE's mission for energy security. This project combines a unique mathematical modeling capability developed at Lawrence Berkeley National Laboratory (LBNL) with oil company experience and expertise to solve the problem. The key to success of this technology is the development of efficient computational models which will be used to calculate flow properties including permeability, capillary pressure, relative permeability, and mechanical properties based on images of the rock pore space derived from cuttings. This direct calculation takes into account the effect of microscale heterogeneity, thereby mitigating one of the major sources of uncertainty in currently available cuttings analysis methods. The needed highly efficient computational models for flow are made possible by innovative application of graph theory, an established branch of topology. Other simple, inexpensive, direct, and indirect measurements of drill cuttings properties, which are available or under development, will be combined with the algorithms developed in this project. The objective of the project is to bring the technology to the point needed for commercialization. Development of the graph theory based computer model for calculation for flow properties has been completed. Final validation of the algorithms by comparison with measurements on a reference suite of samples is underway. This computational system gives a model which can calculate pressure as well as intrinsic and relative permeability when given input parameters describing the statistical properties of the pore geometry. A series of numerical simulations of 2D and 3D salt structures has shown that MT should be able to map the base of salt structures. For field testing, a hardware package to acquire MT data from the sea floor was developed at Scripps, and data processing software was developed at LBNL and University of California at Berkeley. Initial field surveys have been conducted at two sites in the Gulf of Mexico. The first survey, conducted in August 1996 went well but the data were too noisy to be useful. The second survey, conducted in July 1997 after instrument problems were corrected, went extremely well, providing impressive imaging of salt shapes using new numerical codes developed for the project. Oil exploration companies are very interested in commercializing the results of this project. This project supports the DOE mission in energy security.

**74. Title: Advanced Computational Tools for 3-D Seismic Analysis.****ID:** ORL-ACTI-95-09**PI:** Jacob Barhen  
Computer Science and Mathematics Division.**Phone:** 423 574-7131**Partners:** DeepLook (Includes: BP, Chevron, Mobil, Phillips, Shell, Texaco, and UNOCAL)  
Houston, TexasParadigm Geophysical  
Houston, Texas**FY 98 Funding:** \$42K**Total Project Funds:** \$400K

The goal of this project is to develop advanced computational tools (TRUST and DeepNet) that are targeted at a core mission of DOE: to reduce dependence on imported oil by identifying the location of the remaining domestic oil. TRUST is a revolutionary tool for solving global optimization problems that has been applied to the task of focusing underground seismic images (the residual statics problem). Clearly, a sharper image enables the identification of remaining oil. DeepNet is an ultra fast method for training a neural net in which a sequence of alternating direction singular value decompositions is combined with weight renormalizations to minimize the learning error in a single iteration. DeepNet is being applied to a data fusion project that has been defined by DeepLook. The long term DeepLook objective is to fuse data from well logs, core samples, seismic images, and oil production to forecast the position and volume of the remaining oil in an oil field. Neural nets are an outstanding method for data fusion, and DeepNet can reduce the training time by more than an order of magnitude. For the global optimization problem, Paradigm Geophysical provided a computer code to evaluate the objective function (stack power energy) and a sequence of test problems (each problem more difficult than the last). The test problems were so challenging that many fundamental improvements in TRUST were required to solve them. Major accomplishments were: an invention disclosure in 1996, an article in Science Magazine in 1997, and an R&D 100 Award in 1998. For the neural net problem, DeepLook has provided a detailed data base for an oil field. The goal of the first phase of our research is to train neural nets with inputs of seismic data that can forecast the parameters measured in well logs for all parts of the oil field. The next phases will fuse more data and forecast remaining oil.



R&amp;D 100 Award Winner 1998

**American Textiles (AMTEX) Partnership****75. Title: Electrodialysis for Salt Recovery and Reuse****ID:** ANL-AMTEX 2**PI:** Shih-Perng Tsai  
Energy Systems Division**Phone:** 630 252-5006**Partner:** Institute of Textile Technology  
Spartanburg, South Carolina**FY 98 Funding:** \$200K

The goal of this project, as part of the Textile Resource Conservation Project, is to develop electrodialysis processes for the recovery and reuse of salts from dyebath effluents. The U.S. textile industry uses 800 million lb/yr of sodium chloride and sodium sulfate, mostly in dyeing processes. These salts are not consumed during the processes and remain in dyebath effluents. A typical dyeing and finishing plant discharges about 20 million lb/yr of salts. This results in the loss of the salt value and high costs in environmental compliance. Thus, there is a significant opportunity to apply efficient and cost-effective separation technologies to recover the salts for reuse. Argonne National Laboratory is developing electrodialysis processes for the recovery of salts from dyebath effluents. Electrodialysis uses selective permeability of ion-exchange membranes to purify and concentrate ionized species from aqueous streams. In Argonne's process, the salt present in the dyebath effluents is separated from unused dyes and other chemicals, and a brine solution is generated for reuse in making new dyebaths. This enables reuse of salt, lowers a textile plant's operating costs, and eliminates an unwanted discharge into the environment. It can have a tremendous effect on increasing the competitiveness of the textile industry while reducing the environmental impact of its operation. Laboratory scale electrodialysis experiments have been conducted since 1994, with simulated and actual dyebath effluents. The process feasibility was demonstrated, and suitable technical parameters and process conditions were established. The laboratory results showed that up to 95% of salt can be recovered from treated dyebath effluents, a concentrated good purity brine can be generated for reuse, and the energy consumption is economical. The project is currently performing a pilot-scale field demonstration at a mill for scale up and brine reuse tests. A host mill site has been selected, and preparations for the field tests are underway. The field demonstration is planned to start in late 1998. The electrodialysis technologies being applied to the textile industry for salt recovery have applications in other processing industries for pollution prevention and efficient product separation. Several such applications are being developed in DOE sponsored programs for the chemical, agriprocessing, and forest products industries. The technology advancement and field experience

from this work will significantly benefit these programs. The electrodialysis technologies also have applications in DOE environmental remediation and restoration programs.

**76. Title: Synthesis of Carboxymethylcellulose from Waste Fabric**

**ID:** ANL-AMTEX 4

**PI:** Yuval Halpern  
Energy Systems Division

**Phone:** 630 252-2908

**Partner:** Institute of Textile Technology  
Spartanburg, South Carolina

**FY 98 Funding:** \$95K

The textile industry produces large quantities of waste cotton and cotton/poly-ethyleneterephthalate (PET) blend fabric. Disposal of this waste (either by incineration or landfilling) is a costly operation. With tighter regulations and less air space available in landfills, the cost of disposal continues to rise. On the other hand, the textile industry buys large amounts of carboxymethylcellulose (CMC) which is used as a sizing agent in the slashing operation. The starting material for CMC is cellulose (mostly wood cellulose). While cotton/PET blend fabric waste contains large quantities of cellulose, cotton fabric waste is practically pure cellulose. It is logical to try to convert the textile industry's cotton containing waste into a useful sizing agent, which supports DOE's mission to reduce waste streams in the major energy-consuming industrial sectors. Small scale, preliminary results at Argonne National Laboratory (ANL) showed the technical feasibility of such a conversion. In order to evaluate the produced CMC as a sizing agent, and to get insight into the economics of the conversion process, enough CMC had to be prepared from various types of waste fabric. Six types of waste cotton fabric were selected for the conversion to CMC: prepared cotton; light vat-dyed without finish; light vat-dyed with finish; reactive-dyed without finish; reactive-dyed with finish; and indigo-dyed without finish. A medium scale reaction process was developed at ANL, and 600 g of CMC were prepared from each of the above waste types. Each of the CMC products was evaluated as a sizing agent and compared to commercial CMC for the following properties: degree of substitution (DS); viscosity of dilute water solution; sized yarn strength; percent size add-on; yarn encapsulation; and Reutlinger Webster ST-6 abrasion resistance. For all waste converted to CMC (except that from reactive-dyed with finish fabric), the evaluated properties were as good as or better than those of the commercial CMC size. It was established that high quality CMC size can be produced from waste cotton fabric.



**77. Title: Sensing and Reduction of Air Emissions****ID:** ANL-AMTEX 5**PI:** C. David Livengood  
Energy Systems Division**Phone:** 630 252-3737**Partner:** Institute of Textile Technology  
Spartanburg, South Carolina**FY 98 Funding:** \$50K

Textile industry plants have the potential to emit a wide variety of airborne chemical species from various stacks and vents. These species arise from the application and subsequent processing of the formulations needed in the manufacture of fabric and fabric products, as well as from a multitude of combustion sources used to generate process heat. In general, these emissions have not been well characterized, with the quantities of most species being estimated on the basis of simple mass balances. Both process control and environmental permitting activities would benefit from the ability to economically and accurately monitor those species that have the greatest regulatory concern and/or process-control implications. In consultation with industry representatives, formaldehyde was selected for study in this project. The initial objectives of this project were twofold. In the short term, commercial formaldehyde monitors that might serve immediate industry needs were surveyed and evaluated. Two instruments were selected for field evaluation. For the longer term, the project participated in the further development of solid-state sensors based on a ceramic-metallic (CERMET) "sandwich" concept. This concept offered the promise of rugged, low-cost, low-power sensors that could be used for continuous monitoring of critical process effluents. The construction and operation of the sensors were optimized in the laboratory for chemicals of interest to the textile industry, and one sensor was given a brief field test. In the project, evaluation of emissions from various textile processes became a third objective that extended beyond simply testing sensors. Two field campaigns were conducted at different facilities, with the second involving measurement of emissions from three different processes. The final report for the project will describe the commercial monitors that were identified and the performance of the units tested in the field, detail the CERMET sensor development activities and laboratory testing, and summarize the field-test results for the sensors and process-emissions measurements. This project supports the DOE objective of improving the energy/environmental performance of the U.S. textile industry and thereby enhancing the international competitiveness of the industry.

**78. Title: Computer-Aided Fabric Evaluation (CAFE)****ID:** ORL-AMTEX 6**PI:** Glenn O. Allgood  
Instrumentation and Controls Division**Phone:** 423 574-5673**Partner:** Institute of Textile Technology  
Spartanburg, South Carolina**FY 98 Funding:** \$525K

Currently the U.S. textile market is under pressure from offshore competition to reduce product costs and enhance quality. Since their operating and support costs are fixed, they are forced to find alternative means to accomplish this. One is through technology innovation that increases process efficiency without impacting plant performance, i.e., technologies that meet stringent economic and functional requirements. This is the focus of the CAFE Project. The particular area of need is fabric inspection. The specific requirements are to develop systems, methods, and approaches that inspect cloth for structure and optical flaws and provide process information as it relates to the construction. These requirements dictate that inspection and analysis be performed close to the point of fabric formation, i.e., on-loom and in the print lay-down area. In addition to this, CAFE was asked to develop a machine diagnostic capability to identify machine problems that contribute to product off-quality. Given these needs, the CAFE project has developed and delivered to the CAFE industry partners four specific technological innovations. The first is the CAFE Economic Model which has been used to determine the economic viability of CAFE technologies and total impact on the manufacturing infrastructure. Technologies that have been developed to support fabric and color inspection include a Pick Measurement Device and an Imaging Colorimetry System. The Pick Measurement Device is a laser-based system that provides information about fabric construction (density, total picks, and process information). The first generation system was delivered in 1996. A beta version was delivered for compliance testing this year. It is currently undergoing algorithm modification to allow it to detect and qualify fabric anomalies. The proof-of-concept Colorimetry System is being developed this year. It will provide a novel color transform that is more closely aligned with the human vision system. Machine Diagnostics is a task that was completed last year and submitted as one of the project's deliverables. The DOE has found that this capability can be used to enhance their production facilities and has funded as a deployment task. The benefits to DOE will be in the application of the Economic Model to a value chain analysis for the steel industry, application of the Colorimetry System in biological studies, deployment of the Pick Measurement Device for metrology and material construction, and the deployment of Machine Diagnostics in facilities, both currently operating or those in standby status.

**79. Title: Technology Resource Conservation Environmental Decision Tools****ID:** PNL-AMTEX 1**PI:** Tapio Kuusinen  
Environmental Technology Division**Phone:** 509 372-4234**Partner:** Institute of Textile Technology (ITT)  
Spartanburg, South Carolina**Phone:** 864 595-0035**FY 98 Funding** \$145K

To be competitive in the international marketplace, textile manufacturers must produce superior products that are delivered on time and produced with minimum cost and liability. Unfortunately, many of the largest opportunity costs are hidden, as they have been incorporated into operating standards or exist due to historical industry practices. Many of these hidden costs in the textile chain are in the environmental and energy areas. Advanced decision systems, or tools, are increasingly important as business and environmental decisions become more complex and interrelated. While business and environmental decisions are becoming more complex, the corporate down-sizing trend in U.S. industry leaves fewer and fewer people to make more complex decisions. Environmental decision tools developed in this project will provide the opportunity for textile companies to more thoroughly evaluate the environmental and cost consequences of business decisions. Textile environmental decision tool development was initiated at Pacific Northwest National Laboratory (PNNL) in 1995 with funding received from the Environmental Protection Agency (EPA). Two prototype software products were subsequently developed: the Textile Resource Integration Model (TRIM), and the Pollution Prevention Design Guidelines for Engineers (P2EDGE) Model. TRIM is an analytical tool that allows a product or process designer to understand the economic and life-cycle environmental consequences of design alternatives. P2EDGE-Textile helps industrial product and process designers identify pollution prevention opportunities within their company and plants. Both of these software products support the DOE missions of reducing industrial energy consumption and pollution. In this project, distribution and user support strategies will be developed for application of TRIM and P2EDGE by Textile Resource Conservation (TReC) member companies. Plans are to commercialize the textile industry version of P2EDGE through ITT. The commercial version of TRIM, known as LC Advantage, also will be distributed through ITT. Additionally, LC Advantage is being made available commercially to other industrial sectors via Battelle Press, and also is the recipient of a 1998 R&D 100 Award. Work also



R&amp;D 100 Award Winner 1998

has been initiated on a third TReC environmental decision tool product, a prototype software application that will allow users to incorporate environmental considerations into the selection of textile colorant systems. The selection of colors used in producing textile products can have a significant impact on the environmental and resource efficiency implications of the dyeing process. However, tools to assist the designer in making these comparisons do not currently exist. The development of this capability will also support the DOE mission of reducing industrial energy consumption and pollution.



**80. Title: Carbon Dioxide Based Sizing and Desizing (Slashing)**

**ID:** PNL-AMTEX 3

**PI:** Larry E. Bowman  
Environmental and Health Sciences Division

**Phone:** 509 375-1066

**Partner:** Institute of Textile Technology  
Charlottesville, Virginia

**FY 98 Funding:** \$235K

Conventional methods for textile sizing and desizing (also known as slashing) consume a large amount of energy and generate a significant volume of waste water. Prior to weaving, size is added to yarn using a water solution, and the yarn is dried before it is woven. Desizing of the woven fabric generates a large volume of waste water containing the spent size material. Pacific Northwest National Laboratory (PNNL), in conjunction with the Institute of Textile Technology (ITT) and their AMTEX partners, is developing a new sizing and desizing technology that consumes much less energy and generates virtually no waste. Implementation of this process would be a significant step toward making modern textile manufacturing energy efficient and "zero discharge." Based on previous work, PNNL has developed a new class of size materials that are soluble in supercritical or liquid carbon dioxide. In a small weaving trial at ITT, these size materials provided equivalent or superior abrasion resistance compared with conventional size. The objective of this project is to develop sizing and desizing methods that allow these size materials to be used for weaving cotton/polyester blends and then be recovered and reused. Two application methods are being investigated: electrostatically-assisted deposition of powdered size and immersion in a solution of size in liquid carbon dioxide. PNNL will size a small warp by each method, and ITT will conduct weaving

trials. PNNL will also desize the woven fabric using liquid carbon dioxide. The benefits to DOE would be the significant energy savings and waste reduction that would accrue following commercial implementation of this technology.

**EXAMPLES OF RAPID ACCESS PROJECTS****Personnel Exchange****81. Title: Optimized Catalysts for the Cracking of Heavier Petroleum Feedstocks****ID:** LBL98-PX-17**PI:** Gabor Somorjai  
Materials Sciences Division**Phone:** 510 642-4053**Partner:** Catalytica, Inc.  
Mountain View, California**FY 98 Funding:** \$40K

Catalysts lower the energy required for chemical reactions to proceed and are widely used in petroleum refining and chemical manufacturing. The useful lifetime and, thus, the value of an industrial catalyst are limited by a process called deactivation in which the efficiency of the catalyst declines over time. Understanding this deactivation process is essential for developing new catalysts with longer useful lifetimes. The objective of this project is to develop a new surface science tool, ultraviolet (UV) Raman spectroscopy, that can identify chemical species on the surfaces of catalysts in situ under actual reaction conditions. In collaboration with Catalytica, the project will apply this tool to study an important class of catalysts used in petroleum refining. The initial catalytic system to be studied will be zeolite catalysts used in the "cracking" reactions that produce high octane gasoline from petroleum feedstocks by converting heavier hydrocarbons to lighter species. A combined reactor - UV Raman system was constructed at Lawrence Berkeley National Laboratory. By monitoring spectroscopically the identity of the surface species in real time, the project will determine the precise mechanism by which deactivation occurs and so-called "additives" and "promoters" inhibit or reverse catalyst deactivation in this system. For initial experiments, Catalytica chose two commercially available zeolite catalysts used for petroleum cracking. Initial results indicate that high quality UV Raman spectra can be obtained, far superior to those results obtained from conventional Raman spectroscopy.

**Technical Assistance****82. Title: Waste Stabilization of Foundry Preparations****ID:** ANL98-TA-83**PI:** K. C. Goretta  
Energy Technology Division**Phone:** 630 252-7761**Partner:** The Raven Group  
Casper, Wyoming**FY 98 Funding:** \$3K

This project has identified a need for stabilization of heavy-metal-contaminated sand from local foundry operations. Pb and Cd are of greatest concern. Raven has a second goal of making useful byproducts, such as aggregates, from the stabilized waste forms. Argonne National Laboratory's proprietary Ceramicrete binders will be used to accomplish the stabilization and to fabricate dense, strong forms that can be used as value-added products. The key challenge will be to develop a binder that can meet cost restrictions. Economic analysis was conducted to determine the cost of the Ceramicrete binder relative to other process and product costs. The project's basic formulation appeared to be too expensive. The project identified substitution of sodium for the potassium in the current formulation as the best way to reduce costs while maintaining good stabilization. A new formulation for Ceramicrete was developed, and instructions for how to apply it were supplied to Raven. Work is now in progress at Raven to evaluate the effectiveness of the new binder system, to determine the properties of the stabilized waste forms, and to assess the applicability of these forms to various end-use products. The best benefit to be derived from this project would be elimination of a serious environmental problem by recycling waste. Furthermore, the stabilized products produced should have inherent value as, perhaps, a stable aggregate added to other products. DOE's mission to integrate environmental research, development, assessment, and remediation supports this project's objectives.

**83. Title: Analysis of Personal Computer Platform Software****ID:** ANL98-TA-86**PI:** Keng Leong  
Technology Development Division**Phone:** 630 252-3254**Partner:** Spawr Industries  
Lake Havasu City, Arizona**FY 98 Funding:** \$4K

The objective of this project is to assist Spawr Industries in the development of a personal computer (PC)-based data acquisition and analysis system for Argonne National Laboratory (ANL) weld monitoring technology that has been licensed to Spawr Industries. The project has provided Spawr with insight into analysis requirements for the weld monitor data in real world conditions. Details of the analysis procedures were provided to Spawr. The ANL principal investigator visited Spawr Industries to examine the software system they developed using National Instruments' Laboratory View Application. Suggestions for improvements in the analysis routines were made. The result of the effort was the development of a complete weld monitoring system, i.e., hardware and software which helped to convince potential users of the viability of Spawr's monitoring system. As a result, six new orders were received from an automotive company. It is expected that with the acceptance of Spawr's monitoring system, weld monitoring will become a standard at automotive manufacturing plants, and the cost and quality of products will improve. The development of a robust weld monitor system with software for analysis and defect detection will spur sales of the monitor system. The implementation of such systems in manufacturing will increase the quality and manufacturing efficiency.



**SMALL CRADAs****84. Title: Development and Validation of Computational Fluid Dynamics Simulation of a Novel Fluid Catalytic Cracker Process****ID:** ANL98-SC-06**PI:** S. L. Chang  
Energy Systems Division**Phone:** 630 252-6955**Partners:** Process Innovators, Inc.  
Salt Lake City, Utah**FY 98 Funding:** \$40K

Process Innovators, Inc. (PII) is developing a staged, fluid catalytic cracking process, referred to as the Low Profile Fluidized Catalytic Cracker (LPFCC), that has the potential to substantially and positively impact critical Fluid Catalytic Cracker (FCC) performance indices, namely, product selectivity, operating flexibility, throughput, reliability, operating cost, and emissions. The primary goal of this project is to accelerate the development and commercialization of a novel, staged FCC process through the application of computational fluid dynamic (CFD) analytical methodologies for analyzing and interpreting data derived from a small-scale, 1000 bbl/day demonstration unit. PII is building the 1000 bbl/day LPFCC Commercial Demonstration Unit at the Flying J Refinery; the unit will be dedicated to this project. The validated CFD simulation of the FCC will provide PII with the sound technical basis needed to overcome the major commercialization barrier, namely, the reluctance of a conservative industry to accept novel technology that is not thoroughly proven. Argonne National Laboratory acquired the information for the CFD simulation of the pilot-scale LPFCC unit from PII. The information provided by PII includes the riser dimensions, the flow rates of catalyst, oil, and lift gas, and the operating temperature and pressure of the LPFCC unit. After resolving the numerical problems, preliminary calculations of the multiphase non-reacting flow were performed. This project contributes to DOE's strategic objective to help develop, test, and demonstrate novel/improved technologies that reduce energy consumption and environmental emissions.

**85. Title: Microcooling Systems for Thermal Control****ID:** LBL98-SC-22**PI:** Keith Jackson  
Materials Sciences Division**Phone:** 510 486-6894**Partners:** Saddleback Aerospace  
Los Alamitos, CaliforniaX-Form Corporation  
Rohnert Park, California**FY 98 Funding: \$100K**

The control and removal of heat from high power density components, especially where uniform temperatures must be maintained, is a major limiting factor in many applications, including heat removal from integrated circuits, the efficient operation of high power laser systems, and prevention of thermal distortion in beamline optics. In addition, the thermal dissipation demands new approaches that push the limits of thermophysics knowledge. It is particularly challenging to maintain a temperature of less than 100 deg C from a system volume less than 0.001 liters with heat transfers of several hundred kilowatts (high-efficiency microsystems cooling). Indeed, thermal control for microsystems enters into a new thermophysics regime that has yet to be tested and explored. The approach we are applying is passive cooling. Passive structures such as electronic heat sinks allow heat to dissipate into the ambient environment through natural convection. Micro-fabricated passive elements have surface area-to-volume ratio and fin densities over one order of magnitude higher than currently available. Microchannels have excellent heat transfer capabilities; typically a microchannel cooler can achieve a 20-fold decrease in thermal resistance as compared with a conventional water-cooled heat sink. Batch replication of these microstructures would allow large surface area cooling through arrays of modules, and drive down costs relative to conventional machining technologies. To explore the thermo-physical limits of passive systems, LIGA (Lithography, Galvanoformung [Electroplating], Abformung [Molding]), are used to fabricate the components for the proposed micro-cooling system. LIGA is a series of process steps with unique results: fabrication of metallic structures; aspect ratios surpassing 100:1 (demonstrated at 14 um feature size); structure heights up to several millimeters; high precision in sidewall verticality and finish (less than 0.05 mrad divergence and 20 um roughness); and feature sizes down to 2 um. Batch replication is achieved using etched and electroplated structures to serve as molds in future processing. The Advanced Light Source is used to provide the bright x-ray light required for the LIGA beamline/scanner.

## APPENDIX A

## CROSS REFERENCE TABLE FOR MULTI-YEAR PROJECTS\*

| Program Focus Area                                       | ANL        | BNL            | LBNL       | ORNL               | PNNL       |
|--|------------|----------------|------------|--------------------|------------|
| <b>Advanced Materials</b>                                |            |                |            |                    |            |
| Design of Materials                                      | 1          |                | 2, 3, 4    | 5, 6               | 7, 8       |
| Advanced Synthesis and Characterization Technologies     |            |                | 9, 10      | 11                 |            |
| Films and Coatings                                       | 12, 13     | 14, 15         | 16         | 17, 18             | 19         |
| Energy Conversion and Storage                            | 20, 21     | 22, 23, 24, 25 | 26, 27     | 28                 |            |
| <b>Intelligent Processing and Manufacturing Research</b> |            |                |            |                    |            |
| Intelligent Design                                       | 29         |                |            |                    | 30         |
| Intelligent Manufacturing Processes                      |            | 31             |            | 32, 33, 34, 35, 36 |            |
| Enabling Technologies                                    |            | 37, 38, 39     | 40         | 41, 42, 43, 44     |            |
| <b>Environmental and Biomedical Research</b>             |            |                |            |                    |            |
| Biotechnology  |            |                |            |                    | 45, 46     |
| Medical Technologies                                     | 47         | 48, 49         | 50, 51, 52 | 53, 54             | 55         |
| Cleaner Industrial Processes                             | 56, 57, 58 | 59, 60         | 61         | 62, 63, 64         | 65, 66, 67 |
| Environmental Technologies                               |            | 68             |            |                    | 69         |
| <b>Major Industry Partnerships</b>                       |            |                |            |                    |            |
| Advanced Computational Technology Initiative (ACTI)      | 70         |                | 71, 72, 73 | 74                 |            |
| American Textiles (AMTEX) Partnership                    | 75, 76, 77 |                |            | 78                 | 79, 80     |

\* The numbers in this list refer to the project sequence numbers in this book.

## APPENDIX B

## ALPHABETICAL LIST OF INDUSTRIAL PARTNERS\*

|  |            |
|--|------------|
| AccSys Technology, Inc. ....                           | 48         |
| Advanced Vehicle Systems, Inc. ....                    | 63         |
| Aera Energy ....                                       | 73         |
| Air Products ....                                      | 65         |
| Alumax Corporation ....                                | 41         |
| Amoco Corporation ....                                 | 20-22, 71  |
| Analysis and Design Applications Company (adapco) .... | 29         |
| Applied Science and Technology ....                    | 12         |
| ARCO ....  | 70, 73     |
| Association of American Railroads ....                 | 56         |
| Babcock and Wilcox ....                                | 59         |
| BP Exploration ....                                    | 70         |
| BP-America ....  | 73, 74     |
| Catalytica, Inc. ....                                  | 66, 81     |
| Chattanooga Area Regional Transit Authority ....       | 63         |
| Chevron ....   | 70, 72, 75 |
| Commonwealth Scientific Corporation (CSC) ....         | 10         |
| Conoco ....  | 70         |
| Consolidated Edison ....                               | 59         |
| Continental Optical Corporation ....                   | 37         |
| Corning Inc. ....                                      | 30         |
| Cray Research ....                                     | 70         |
| DeepLook ....  | 75         |
| Diesel Technology Company ....                         | 13         |
| Dow Chemical Company ....                              | 57         |
| DuPont Company ....                                    | 60, 61     |
| Durametallic ....                                      | 12         |
| Electric Transit Vehicle Institute ....                | 63         |
| Electric Power Research Institute ....                 | 19         |
| Electro-Motive Division of General Motors ....         | 56         |
| Energy Research Corporation (ERC) ....                 | 27         |
| Engelhard/ICC ....                                     | 62         |
| eV Products Division of II-VI, Inc. ....               | 38         |
| Exxon ....   | 74         |
| Finkl & Sons Company ....                              | 36         |

\*The numbers in this list refer to the project sequence numbers in this book.

|  |       |
|--|-------|
| Forging Industry Association               | 36    |
| Forrester Environmental Services, Inc.     | 68    |
| Front Edge Technology, Inc.                | 13    |
| General Atomics (GA)                       | 51    |
| Genometrix Inc.                            | 46    |
| Genzyme Corporation                        | 52    |
| Geotools Corporation                       | 74    |
| Gould Electronics, Inc.                    | 25    |
| Grace Construction Products                | 14    |
| Hewlett-Packard Laboratories               | 3     |
| Honeywell Solid State Electronics Center   | 18    |
| Houston Advanced Research Center           | 41    |
| Howmet Corporation                         | 19    |
| Hughes Christiansen                        | 42    |
| IBM  | 9, 68 |
| Implant Innovations, Inc.                  | 55    |
| InnerDyne, Inc.                            | 54    |
| Institute of Textile Technology            | 75-79 |
| International Business Machines            | 30    |
| International Fuel Cells Corporation       | 24    |
| Kaiser Aluminum and Chemical Company       | 41    |
| Landmark Graphics                          | 68    |
| Lear, Inc.                                 | 34    |
| Loral Control Systems                      | 31    |
| Lucent Technologies                        | 11    |
| Magnequench International, Inc.            | 5     |
| Marlow Industries                          | 64    |
| Meridian Oil, Inc.                         | 74    |
| Metal Matrix Composite Castings            | 35    |
| Minnesota Mining and Manufacturing Company | 17    |
| Mobil                                      | 68    |
| Nartron Corporation                        | 63    |
| Nonvolatile Electronics, Inc.              | 18    |
| NWG Associates                             | 74    |
| NZ Applied Technologies                    | 4     |
| Oncogene Research Products                 | 49    |
| Oxford Superconducting Technology          | 15    |
| Paradigm Geophysical                       | 81    |
| Performance Research                       | 33    |
| Perkin Elmer Corporation                   | 44    |
| PerSeptive Biosystems                      | 45    |

|   |            |
|---|------------|
| Phillips Petroleum Company . . . . .                                | 20         |
| Power Conversion, Inc. . . . .                                      | 23         |
| Pratt and Whitney . . . . .   | 6          |
| Praxair, Inc. . . . .   | 2          |
| Process Innovators, Inc. . . . .                                    | 84         |
| Rayovac Corporation . . . . .                                       | 26         |
| Reynolds Metals Company . . . . .                                   | 32, 41     |
| Ross Products Division . . . . .                                    | 7          |
| Saddleback Aerospace . . . . .                                      | 85         |
| Schlumberger-GeoQuest . . . . .                                     | 70         |
| Scientific Software-Intercomp . . . . .                             | 70         |
| Scientific Forming Technologies Corporation . . . . .               | 35         |
| Seagate Technology, Inc . . . . .                                   | 16         |
| SEMATECH . . . . .  | 8          |
| Smith and Nephew . . . . .  | 53         |
| Solar Turbines Inc. . . . .   | 19         |
| Southwire Company . . . . .   | 17         |
| Spawr Industries . . . . .  | 83         |
| Stirling Thermal Motors, Inc. . . . .                               | 13         |
| Sunsoft Corporation . . . . .                                       | 50         |
| Supercomputer Automotive Applications Partnership (SCAAP) . . . . . | 29         |
| Superconductive Components, Inc. . . . .                            | 1          |
| Symbol Technologies, Inc. . . . .                                   | 39         |
| Teledyne Electronic Technologies . . . . .                          | 28         |
| Texaco . . . . .  | 68-74      |
| The Raven Group . . . . .   | 82         |
| United Technologies, Inc. . . . .                                   | 58         |
| United Defense, LP . . . . .  | 36         |
| Unocal . . . . .  | 68-74      |
| UOP Research Center . . . . .                                       | 20, 58, 67 |
| USCAR . . . . .   | 69         |
| Waters Corporation . . . . .  | 43         |
| Western Atlas Logging Services (WALS) . . . . .                     | 40         |
| X-Form Corporation . . . . .  | 85         |
| Zimmer, Inc. . . . .  | 47         |

## APPENDIX C

## ALPHABETICAL LIST OF PRINCIPAL INVESTIGATORS\*

|                            |       |
|----------------------------|-------|
| Adams, Donald J. ....      | 63    |
| Adzic, Radoslav ....       | 244   |
| Ahluwalia, Rajesh ....     | 200   |
| Allgood, Glenn O. ....     | 78    |
| Anders, Andre ....         | 10    |
| Anderson, Carl W. ....     | 49    |
| Armstrong, Timothy ....    | 65    |
| Barhen, Jacob ....         | 74    |
| Baskaran, Suresh ....      | 8     |
| Bates, John B. ....        | 28    |
| Bertozzi, Carolyn ....     | 50    |
| Bissell, Mina ....         | 52    |
| Blue, Craig A. ....        | 36    |
| Bowman, Larry E. ....      | 80    |
| Bullock, R. Morris ....    | 60    |
| Butcher, Thomas ....       | 59    |
| Butler, William H. ....    | 18    |
| Cairns, Elton ....         | 26-27 |
| Campbell, Allison A. ....  | 7, 55 |
| Chandler, Darrell P. ....  | 45-46 |
| Chang, S. L. ....          | 84    |
| Christen, David K. ....    | 17    |
| Chu, William ....          | 51    |
| Courtright, Edward L. .... | 19    |
| Crabtree, George ....      | 1     |
| Ellingson, William A. .... | 47    |
| Erdemir, Ali ....          | 13    |
| Fairchild, Phillip D. .... | 62    |
| Fann, George ....          | 30    |
| Francis, A.J. ....         | 68    |
| Goretta, K. C. ....        | 82    |
| Haller, Eugene ....        | 3     |
| Halpern, Yuval ....        | 76    |
| Hansen, James R. ....      | 35    |
| Hayden, H. Wayne. ....     | 32    |

\*The numbers in this list refer to the project sequence numbers in this book.

|                            |        |
|----------------------------|--------|
| Haynes, Tony E. ....       | 11     |
| Holcomb, David E. ....     | 42     |
| Horton, Joseph A. ....     | 5      |
| Isaacs, Hugh ....          | 14     |
| Jackson, Keith ....        | 85     |
| Jorgensen, James D. ....   | 21     |
| Kenik, Edward A. ....      | 6      |
| Knapp, Jr., F. F. ....     | 54     |
| Krauss, Alan ....          | 12     |
| Kuusinen, Tapio ....       | 79     |
| Lauf, Robert J. ....       | 33     |
| Lee, Ki Ha ....            | 40     |
| Leong , Keng ....          | 83     |
| Livengood, C. David ....   | 77     |
| Mahajan, Devinder ....     | 22     |
| McBreen, James ....        | 23     |
| McMillan, A. D. ....       | 53     |
| Morgan, Tom ....           | 70     |
| Morrison, H. Frank ....    | 74     |
| Myer, Larry R. ....        | 73     |
| Nicholas, John ....        | 66     |
| O'Connor, Paul ....        | 38-39  |
| Orlando, Thomas ....       | 69     |
| Padmore, Howard ....       | 9      |
| Patzek, Tad ....           | 73     |
| Pellin, Michael J. ....    | 57     |
| Ramsey, J. Michael ....    | 43     |
| Sales, Brian C. ....       | 62     |
| Salmeron, Miquel ....      | 16     |
| Schlyer, David J. ....     | 48     |
| Sekar, Raj ....            | 56     |
| Simpson, Michael L. ....   | 44     |
| Somorjai, Gabor A. ....    | 61, 79 |
| St. Martin, Edward J. .... | 58     |
| Suenaga, M. ....           | 15     |
| Takacs, Peter Z. ....      | 37     |
| Tsai, Shih-Perng ....      | 75     |
| Visco, Steven ....         | 2      |
| Wang, Yong ....            | 67     |
| Warren, John B. ....       | 31     |



|                       |    |
|-----------------------|----|
| Weber, David P. ....  | 29 |
| Xiang, Xiao-Dong .... | 4  |
| Yang, X.Q. ....       | 25 |
| Young, Jack P. ....   | 41 |
| Zacharia, Thomas .... | 34 |