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LABORATORY TECHNOLOGY RESEARCH

Abstracts of FY 1996 Projects

U. S. Department of Energy
Office of Energy Research
Office of Computational and Technology Research
Advanced Energy Projects and Technology Research Division

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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 Energy Research (ER) multi-program national laboratories and the unparalleled entrepreneurial spirit of American industry.

A distinguishing feature of the ER multi-program national 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 scientific impact of the LTR program has already been dramatic. Since its inception in 1992, the program's technologies have won 12 R&D-100 Awards, 15 Federal Laboratory Consortium Awards, and seven 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 are conducted by the five ER multi-program laboratories: Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge, and Pacific Northwest National Laboratories. These projects explore the applications of basic research advances relevant to Department of Energy's (DOE) mission over a full range of scientific disciplines. The program presently emphasizes three critical areas of mission-related research: advanced materials, intelligent processing/manufacturing research, and sustainable environments.

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.

- Intelligent Design of Materials: Emphasis is placed on modeling and characterization; alloying and doping; composite and functional graded materials; biomaterials; and nanostructures and films.

- Advanced Synthesis 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.

- Intelligent or Adaptive Materials: Emphasis is placed on developing materials that respond to external stimuli, such as shape memory alloys, and magneto-resistant, piezoelectric, and electro-rheologic materials.

Intelligent Processing/Manufacturing Research

Intelligent Processing/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. Much of the work performed under IPMR will ultimately lead to applications in private industry.

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 three 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.

Sustainable Environments

A new generation of environmental technologies is needed that supports pollution prevention, efficient resource use, and industrial ecology. Such technologies can help companies become more competitive by lowering resource and energy needs, reducing waste and emissions control costs, and fostering sustainable development. ER 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 the sustainable environments area stress technologies that emphasize sustainable use of natural resources and avoidance of environmental harm. These may include technologies to control and minimize environmental harm (particularly hazardous wastes), an improved environmental technologies information infrastructure, monitoring technologies, and remediation technologies focused on areas such as manufacturing, transportation, materials, water, and energy.

Research on sustainable environments focuses on three 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, microbiology, and biomedicine fall into this category. A potential area for investigation may be the application of extremophile bacteria to the degradation of toxic wastes.
- Chemical Process Modeling: This area fosters teaming with the Mathematical, Information, and Computational Sciences Division (MICS) of the DOE Office of Computational and Technology Research to apply modeling and simulation capability in development of environmentally benign chemical processes. This topic may span a spectrum from the application of modeling tools in the development, at the structural level, of new classes of catalysts, to large scale industrial process modeling.

- Novel Energy Devices: New developments in mechanical engineering and materials sciences are progressing toward the miniaturization of motors, pumps, and compressors to a microscale. Further investigation is required to make these devices economically feasible. This area has potential to revolutionize the way heating and cooling are produced and used in commercial and home settings.

PROGRAM IMPLEMENTATION

The LTR program conducts research using three different mechanisms:

- **Multi-Year Projects.** These cost-shared projects between ER multi-program laboratories and private industry are performed in support of DOE missions but also are relevant to industry needs. LTR program funding to ER 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. These projects undergo a competitive review and are selected on the basis of scientific/technical merit and commercial potential.

  All of the multi-year projects which received Fiscal Year 1996 funding from the LTR program (Total = $25.7 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.

- **Quick Response Projects.** These projects provide private industry, especially small businesses, with a means to solve difficult technical problems rapidly by tapping the unique expertise of ER 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 ER laboratories from $3,000 to $100,000 per project.

  Examples of each type of quick response project are included in this book of abstracts. The total funding for quick response projects was $0.9 million in FY 1996.

- **Major Industry Partnerships.** These partnerships team scientists and engineers in DOE national laboratories with an industry sector to research generic problems facing the industry. The LTR program supports the American Textiles (AMTEX) Partnership and the Advanced Computational Technology Initiative (ACTI) Partnership. The objective of AMTEX is to transfer advanced technology into the Integrated Textile and Apparel sector. ACTI focuses on the discovery and recovery of oil and gas by supporting borehole seismic, oil recovery, drilling and completion, and computational technologies. In both partnerships, DOE and industry research generic, pre-competitive technologies for their mutual benefit. DOE supports national laboratory scientists and engineers, and industry supports its own researchers.

Major industry partnership projects funded by the LTR program 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 1996 funding from the LTR program, are listed as project sequence numbers 103 - 109. For information on the AMTEX program, contact the AMTEX Laboratory Program Office at the Oak Ridge Y-12 Plant, Oak Ridge, Tennessee, 37831, Telephone (423)576-5526.

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ABSTRACTS OF MULTI-YEAR PROJECTS SUPPORTED IN FY 1996

ADVANCED MATERIALS

Synthesis and Processing

1. Title: Cold Cathode Electron Emission from Diamond and Diamond-Like Carbon Thin Films for Flat Panel Computer Displays

ID: ANL95-02

PI: Alan Krauss
Materials Sciences Division

Phone: 708 252-3520

Partner: SI Diamond Technology, Inc.
2345 North Boulevard
Houston, TX

FY 96 Funding: $140K **Total Project Funds:** $420K

Cold cathode electron emission has been observed from a number of diamond and diamond-like carbon thin films. It is expected that this phenomenon can be used for the development of high visibility displays for critical applications such as avionics, high reliability microelectronics applications for operation in harsh environments where maintenance is not feasible, and flat panel computer displays. In this latter application, it is expected that cold cathode emission technology will result in a significant reduction of plant cost, unit cost, and energy consumption compared with current active matrix liquid crystal (AMLCD) displays. Development of diamond field emission technology for reliable displays will also provide a means for U.S. industry to enter the multi-billion dollar flat panel display market which is currently dominated by Asian industries. However, several of the key physical properties which affect field emission performance are normally interrelated so that it is difficult to perform controlled measurements of the effects of these properties on electron emission. The development of devices like flat panel computer displays which use cold cathode electron emission has been hampered by a lack of basic understanding of the emission process. A method has been developed at ANL for the growth of diamond films in the near-absence of atomic hydrogen, using Ar-C60 or Ar-CH4 plasmas. This method produces films which respond differently to variations in growth conditions compared with films grown in large quantities of hydrogen. The differences manifest themselves in the manner in which the nucleation density, grain size, grain boundary width, surface roughness, crystallographic orientation and the extent and localization of regions of sp2 and sp3 electronic bonding character vary with the hydrogen concentration in the plasma. We have been able to relate several of these properties to the effective work function, turn-on

voltage and emission site density by comparing the electron emission behavior and physical properties of conventional micro-and nano-crystalline, and low-hydrogen nanocrystalline diamond films.

2. Title: A Giant Magnetoresistance Wire Sensor

ID: ANL95-07

PI: Samuel Bader
Materials Science Division

Phone: 708 252-4960

Partner: Sagax Technology Corporation
4111 Central Ave., N.E.
Columbia Heights, MN

FY 96 Funding: $280K **Total Project Funds:** $800K

Giant Magnetoresistance (GMR) materials are composite metals whose resistance changes in the presence of magnetic fields. These materials are up to one hundred times more sensitive to magnetic fields than previously known systems. Currently the GMR materials are made by thin-film processing techniques thereby making their cost prohibitive for many applications. The goal of this project is to develop giant Magnetoresistance sensors by inexpensive bulk processing techniques such as wire drawing, and to make prototype sensors that could be used in a variety of applications.

3. Title: Development of CdTe/CdZnTe Materials for Radiation Detectors

ID: BNL94-09

PI: Csaba Szeles
Physics Division

Phone: 516 344-3710

Partner: II-VI, Inc.
375 Saxonburg Blvd.
Saxonburg, PA

FY 96 Funding: $208K **Total Project Funds:** $495K

The objective of this project is to broaden and hasten the commercialization of Cadmium Zinc Telluride (CdZnTe) materials as room-temperature solid-state radiation detectors. Achieving this goal requires improvement of the existing material-growth and processing techniques in order to enhance the production yield and energy resolution of CdZnTe crystals limited by the unpredictability of the as-grown material. This unpredictability is largely due to the uncontrolled incorporation of electrically active native and impurity-related defects in the bulk and at the surface of the crystals and defects at the semiconductor-metal interface. Production of better crystals demands improved understanding of the nature of lattice defects, their influence on the detector performance and their formation and compensation mechanism during the crystal growth and processing. The availability of inexpensive, high-efficiency, room-temperature gamma-ray detectors is of great commercial potential. It stimulates instrument and device manufacturers to develop new products and retrofit old applications using conventional NaI(Tl) and HPGe detectors. The total addressable market for CdZnTe materials and the new instruments and devices that integrate CdZnTe as a primary gamma-ray detector is in excess of 40 million dollars annually.

4. Title: High Density Silicon Carbide Ceramics Demonstrated with Microwave Energy

ID: ORL92-07

PI: Harold D. Kimrey
Metals and Ceramics Division

Phone: 423-576-5183

Partner: Dow Chemical Company
Midland, MI

FY 96 Funding: $ 172K **Total Project Funds:** $ 650K

The goal of this project is to determine if there is an advantage to using microwave processing to densify beta silicon carbide. Conventional sintering of beta silicon carbide has been found to be dependent on removing residual SiO_2 on the surfaces of SiC particles. This is typically done by reducing SiO_2 with carbon below a temperature of about 1600 C, which requires the removal of CO. As the thickness of the part increases, the removal of CO becomes slow and obtaining a uniformly dense body becomes difficult. The application of microwave heating during this process may accelerate the removal of CO due to temperature gradients within the part. Part thicknesses are presently limited to about one inch due to the time required to remove this CO. The ability to densify a thicker part would be a desirable outcome of this program. Less conventional sintering of silicon carbide involves the addition of oxides. These typically lower the sintering temperature, which would make them amenable to the present technology of insulating in a microwave furnace.

5. Title: The Growth of Large Single Crystals of MgO

ID: ORL92-22
PI: Lynn A. Boatner
Solid State Division

Phone: 423-574-5492

Partner: Commercial Crystal Laboratories
Naples, FL

FY 96 Funding: $ 115K **Total Project Funds:** $ 325K

The purpose of this partnership is to grow large MgO crystals to be used as substrates in various electronic and optical applications. The technology and experience in growing large crystals will enable Commercial Crystal Laboratories to compete in the international market for these crystal substrates. New high-technology applications for single crystals of magnesium oxide (MgO) in both bulk form and as oriented substrates for the growth of thin films of superconductors and electro-optic materials continue to be identified. For example, MgO single crystals that are grown using the improved techniques developed in the course of this CRADA are presently being used in a new research project that is currently supported by the DOE Office of Nuclear Non-Proliferation (NN-20). The progressive identification of new applications and requirements for MgO single crystals in both DOE project areas and in the commercial realm has resulted in an increasing international market and demand for this material. In the course of this CRADA, progress in realizing major increases in the size of single crystals of MgO produced by means of the submerged-arc fusion-technique has been the result of several significant improvements. These improvements include: A completely new crystal-growth protocol in terms of the processing time and electric arc power, a new graphite-electrode configuration, and the pioneering application of seeding techniques that are based on the formation of a large "mosaic" seed crystal. This new insight into the growth mechanism of MgO from the melt has recently been applied to the formation of a new type of mosaic seed crystal. This new approach to the creation of a mosaic seed represents a much more efficient use of the smaller MgO single-crystal components that are individually oriented and assembled to form the final large composite seed required for use in the arc-fusion crystal-growth method. The initial tests carried out using mosaic seeds fabricated by means of this new approach are very promising and several large MgO single crystals have been grown.

6. Title: Advanced Ceramics for Land Based Gas Turbine Vane Applications

ID: ORL94-19

PI: Joachim H. Schneibel
Metals and Ceramics Division

Phone: 423-576-4644

Partner: Westinghouse Power Generation
Orlando, FL

FY 96 Funding: $80K **Total Project Funds:** $270K

The objective of the project is to examine the feasibility, fabrication, and performance of ceramic or ceramic-composite leading edges for land based turbine vane applications. In order to increase the efficiency of land-based gas turbines, inlet gas temperatures have to be increased, while minimizing the amount of compressor discharge air used for cooling. Presently, thermal barrier coatings (TBC's) are the state of the art in achieving these goals. However, since TBC's are very thin (typically 200-250 mm), they have clear limitations. Since all-ceramic turbine vanes would be a very large and risky development step, Westinghouse is considering the protection of just the leading edges of turbine vanes with high-performance ceramics.

7. Title: Processing Property Relationships in Centrifugally Cast Al-Metal Matrix Composites (MMC)

ID: PNL94-02

PI: Edward Courtright
Material Sciences Division

Phone: 509 375-6926

Partner: General Motors Corporation Gear Center
37350 Ecorse Road
Romulus, MI

FY 96 Funding: $245K **Total Project Funds:** $830K

The goal of this project is to develop cost-effective selectively reinforced metal matrix processing technology. Light alloy metal matrix composites (MMCs) reinforced with silicon carbide or alumina particulates can replace steel in many automobile applications, and the corresponding reduction in vehicle weight translates to a proportional increase in gas mileage. This project concentrates on understanding the microstructure of centrifugally cast MMCs because the process offers the unique capability to distribute the particle phase in regions or zones where the reinforcements will have the greatest benefit. Emphasis will be placed on understanding processing/property relationships and in determining how these can be controlled to optimize selectively reinforced composite structures.

8. Title: Development of Mixed Metal Oxides

ID: PNL94-28

PI: Larry Pederson
Materials and Chemical Sciences Division

Phone: 509 375-2731

Partner: Chemetals, Inc.
711 Pitman Road
Baltimore, MD

FY 96 Funding: $153K **Total Project Funds:** $337K

This project is directed towards the development of unique lithiated metal oxides for use in secondary batteries. The oxides will be produced using PNNL's glycine nitrate process and will involve varying the compositions of the materials to optimize their desired properties. Lithiated manganese oxides are expected to be used in future production of lithium ion systems and the lithium polymer system (which is becoming commercially available with a vanadium oxide cathode). The lithium polymer system is expected to be used as a power source for electric vehicles later in this decade.

9. Title: Innovative Multilayer Thermal Barrier Coatings for Gas Turbine Engines

ID: PNL95-07

PI: Edward Courtright
Materials and Chemical Sciences Division

Phone: 509 375-6926

Partner: Allied Signal, Inc.
111 South 34th Street
Phoenix, AZ

FY 96 Funding: $396K **Total Project Funds:** $835K

The objective of this project is to determine the feasibility of producing innovative multilayer thermal barrier coatings. The fundamental issues associated with maximizing infrared reflectivity and phonon scattering, and the thermodynamic stability issues which affect durability, reliability, and life-cycle performance are being investigated. In the first phase of the program, the feasibility of producing higher performance thermal barrier coatings with multilayered systems will be demonstrated. In the second phase of the program, actual components will be coated and tested by

industrial partners under simulated engine conditions, e.g., burner rigs or in actual land-based gas turbine engines.

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

ID: PNL95-23

PI: Allison Campbell
Materials and Chemical Sciences Division

Phone: 509 375-2180

Partner: Health Tech Development
3845 West Beverly Drive
Dallas, TX

FY 96 Funding: $242K **Total Project Funds:** $597K

The goal of this project is to combine complementary technologies and conduct a testing program which, if successful, would provide information necessary to design and implement a formal development and manufacturing program on novel health-related technology devices for eventual approval by the United States Food and Drug Administration (FDA). If the laboratory research demonstrates that metals or alloys can be reproducibly and uniformly coated using PNNL's unique technology and the biologically suitable metallic or alloy devices coated with the technology are shown to have improved performance in selected animal studies and clinical trials, then the potential products will target a growing market currently estimated to be between $1.2 to $1.5 billion annually.

Materials Design and Characterization

11. Title: Composite Metal-Hydrogen Electrodes for Metal-Hydrogen Batteries

ID: BNL94-06

PI: Myron Strongin
Physics Department

Phone: 516 344-3763

Partner: Energy Conversion Devices, Inc.
1675 West Maple Road
Troy, MI

FY 96 Funding: $254.6K **Total Project Funds:** $699K

The project focuses on the fabrication and characterization of nano-scale bimetallic multilayered films and a feasibility study of their use as hydrogen-containing negative electrodes (anodes) in nickel-metal hydride (NiMH) batteries. If the feasibility of using these new materials is established, it is anticipated that the project will contribute to the advancement of NiMH battery technology and provide batteries with more rapid charging characteristics, greater energy efficiency or larger energy storage capacity.

12. Title: Corrosion Resistance of New Alloys for Biomedical Applications

ID: BNL94-20

PI: Hugh Isaacs
Applied Science Division

Phone: 516 344-4516

Partner: Smith and Nephew Richards Inc.
1450 Brooks Rd.
Memphis, TN

FY 96 Funding: $165K **Total Project Funds:** $450K

The development of new materials for prosthetic devices and other biomedical applications is currently underway. The objective of this project is to provide a detailed understanding of alloy corrosion in bio-systems and the role of the individual alloy additions. Ultimately an understanding of the interactions between alloy composition and the electrochemical response of alloys with optimum mechanical properties and biocompatibility. In situ XANES measurements in simulated bio-

fluid (Ringer's solution) and under crevice conditions (concentrated chloride solution) will provide information on the chemical behavior of the alloys during corrosion. A detailed study of oxide formation will be carried out using XANES, surface analytical techniques and in situ AFM.

13. Title: Nondestructive X-Ray Scattering Characterization of High Temperature Superconducting Wires

ID: BNL95-10

PI: Thomas Thurston
Physics Division

Phone: 516 344-5534

Partner: Intermagnetics General Corporation
4 50 Old Niskayuna Road
Latham, NY

FY 96 Funding: $228K **Total Project Funds:** $630K

Ten years after the discovery of high-temperature superconductors, prototypes of generators, transformers, transmission cables, and current limiters which utilize wires made from these materials are just beginning to be built. The purpose of this CRADA is to characterize the structure of the superconducting material within wires made at IGC in order to understand the causes of poor current carrying capacity, and to suggest alternative processing procedures which can minimize or eliminate the effects which cause poor wire performance. The methods which BNL personnel are using to characterize the wires utilize intense beams of x-rays generated at a special facility at BNL, the National Synchrotron Light Source. Work performed earlier in this CRADA showed that the current carrying capacity is affected by the presence of certain impurity phases, and by poor texturing of the superconducting material within the wires. Both of these deleterious effects can be readily measured only with the intense x-ray beams available at facilities like the National Synchrotron Light Source. Work currently in progress involves direct x-ray monitoring of superconducting wire processing in a "mini-factory" which has been set up at BNL. This work has already suggested modifications to the processing procedures which have helped increase the current carrying capacity of IGC's wires. CRADA personnel have also been characterizing wires made in the DOE's high-temperature superconductor electric power applications program at BNL. Finally, BNL personnel have started to apply the techniques developed to characterize these wires on other problems of interest to the DOE, such as characterizing the properties of battery electrode materials and permanent magnets.

14. Title: A Novel Biocompatible "Smart" Contact Lens Material

ID: LBL94-28

PI: Carolyn Bertozzi
Materials Sciences Division

Phone: 510 643-1682

Partner: Vistakon
P. O. Box 10157
Jacksonville, FL

FY 96 Funding: $245K **Total Project Funds:** $510K

Vision is by far the most important of the human senses and better ophthalmological care products are continuously being sought. For example, current synthetic contact lens materials have limited tolerance by the population. Our goal 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 our design of new contact lens materials, we utilize the lessons we have learned in nature. Our 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 work 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, we focused on carbohydrate molecules which comprise the coating of most living cells. Our strategy, therefore, is to synthesize polymerizable monomers possessing cell surface-like carbohydrates, and to incorporate them into lenses with better biocompatibility properties.

15. Title: Development of Blue-Emitting GaN LEDs and Lasers

ID: LBL94-47

PI: Michael Rubin
Energy and Environment Division

Phone: 510 486-7124

Partner: Hewlett-Packard Laboratories
3500 Deer Creek Road
Palo Alto, CA

FY 96 Funding: $107K **Total Project Funds:** $340K

Efforts in thin film growth led to an improvement of heteroepitaxially grown GaN films to an extent that allows for fabrication of bright ultraviolet and visible light emitting diodes, power devices and lasers. The material's ability to tolerate an unusually large extended defect density allowed for this very rapid technical progress. This project should contribute to the improvement of these devices by: 1) Evaluation of MBE growth of GaN that, by its nature, proceeds far from a thermodynamic equilibrium in contrast to MOVPE or MOCVD GaN thin film growth. The development of a suitable nitrogen source, p-doping of GaN, homoepitaxial growth, strain relaxation and the stoichiometry of GaN are issues, 2) Evaluation of buffer layer growth by laser ablation to provide alternative substrate materials. 3) Evaluation of the atomic scale roughness of surfaces and interfaces that determines the structural film quality and the performance of optical devices if quantum well structures are used.

16. Title: Microscopic Imaging of Magnetic Materials

ID: LBL95-12

PI: Neville Smith
Accelerator and Fusion Division

Phone: 510 486-5423

Partner: IBM Research Center
San Jose, CA

FY 96 Funding: $350K **Total Project Funds:** $1,115K

This project is an IBM-LBNL partnership 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), and to 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. 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. The project combines LBNL's expertise in design and operation of synchrotron instrumentation, beamlines, and experimental end stations with IBM's expertise in microscopy and in the production of artificially engineered magnetic microstructures. 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 the non-volatile magnetic random access memories, and keeping IBM competitive in a fast moving industry.

17. Title: Amorphous Diamond Flat Panel Displays

ID: LBL95-34

PI: Joel Ager
Material Sciences Division

Phone: 510 486-6715

Partner: SI Diamond Technology, Inc.
2345 North Boulevard
Houston, TX

FY 96 Funding: $340K **Total Project Funds:** $596K

The flat panel display market is currently $5 billion/yr and is projected to be as high as $20 billion/yr by 2000 - U.S. companies have less than 5% of the market at present. Displays based on field emission cathodes are a promising alternative technology in which the U.S. currently has a technological head start over the Japanese. SI Diamond Technology (SIDT) has been developing flat panel displays based on field emission from their patented Amorphic Diamond™ material. Although the technology is promising, and SIDT has recently demonstrated a working 3x4" monochrome display, SIDT must solve critical materials problems in their cathode before they can bring mass-produced flat panel displays to market. In the first year of a two-year CRADA project, a team of five MSD PIs has been working with SIDT to understand the structure of their material and its field emission mechanism. SIDT has determined that only a small fraction (<1%) of the cathode area actually emits. In order to improve the emission behavior of the cathodes, the nature of these isolated emission sites, which are embedded in a complex, multiphase matrix, must be understood. In this project, the LBNL strategy is to use measurement expertise in three areas: (1) Raman microprobe spectroscopy, (2) scanning microscopy, and (3) electron microscopy and spectroscopy at the National Center for Electron Microscopy.

18. Title: Alloy Design of Neodymium ($Nd_2Fe_{14}B$) Permanent Magnets

ID: ORL94-15

PI: Joseph A. Horton
Metals and Ceramics Division

Phone: 423 574-5575

Partner: Magnequench International, Inc.
Anderson, IN

FY 96 Funding: $282K **Total Project Funds:** $590K

The objective of this project is to improve the room temperature fracture toughness of neodymium permanent magnets without decreasing their magnetic properties. This will improve machinability, allow closer tolerances, and provide use as a structural element, thus achieving better market penetration for applications such as electric motors. The potential payoff resulting from this project will be a toughened neodymium alloy which displays superior forming properties without sacrificing strength. Market studies predict a substantial growth in the overall neodymium magnet industry from the $750M level today to $5.9B in the year 2000. This rapid commercial growth ensures a continuing high level of interest in new research findings.

19. Title: "Soft" Plasma Cleaning Technology for Semiconductor Processing

ID: ORL94-37

PI: Walter L. Gardner
Fusion Energy Division

Phone: 423-574-1121

Partner: ASTeX
Woburn, MA

FY 96 Funding: $265K **Total Project Funds:** $480K

The objective of this project is the development of a commercially viable, low-temperature process to efficiently remove surface films, principally native oxide, from semiconductor materials while leaving a surface with minimal damage and contamination. The damage and contamination levels should be consistent with the subsequent growth of device-quality epitaxial films and/or deposition of low resistance contacts. A key objective of this project is the evaluation of the effectiveness of unassisted ozone (i.e. without UV radiation) in photoresist removal using high concentrations, up to 10% by weight, of ultra pure ozone produced by an ASTeX Model AX8100 Ozone Generator. Ozone is an established method for removing photoresist from semiconductor wafers that bypasses traditional wet-chemical processing, yet does not introduce oxide damage or mobile ion contamination which may occur with the use of plasma-based stripping tools.

20. Title: Ion Implantation Processing Technologies

ID: ORL94-72

PI: Tony E. Haynes
Solid State Division

Phone: 423 574-2858

Partner: Lucent Technologies - Bell Laboratories
Murray Hill, NJ

FY 96 Funding: $248K **Total Project Funds:** $395K

The objective of this project is to improve ion implantation processing technologies to accelerate the development cycle for two critical technologies required for the manufacturing of the next generation of microelectronic integrated circuits (ICs). These processes include gettering of impurities, where the goal is to identify and evaluate implantation-based schemes for generating stable gettering sites for deleterious impurities within silicon wafers and the problem of transient enhanced diffusion on shallow junction formation. In this project, the feasibility of using ion-implantation-based approaches for solving these problems during manufacturing will be evaluated.

21. Title: Manufacturing of Ni-Base Superalloys with Improved High-Temperature Performance

ID: ORL95-05

PI: C.T. Liu
Metals and Ceramics Division

Phone: 423 574-4459

Partner: Teledyne Allvac
Monroe, NC

FY 96 Funding: $223K **Total Project Funds:** $550K

The objective of this research project is to enhance the manufacturing of high-temperature nickel-base superalloys with improved performance through the control of vital minor elements in the parts-per-million range without significantly increasing production costs. It is anticipated that the control of these vital elements would extend the creep rupture life of superalloy structural members by more than an order of magnitude. Nickel-base superalloys are state-of-the-art materials for high-temperature structural applications in advanced engines, petrochemical, other energy conversion systems.

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

ID: ORL95-07

PI: Kathleen B. Alexander
Metals and Ceramics Division

Phone: 423 574-0631

Partner: Pratt and Whitney
East Hartford, CT

FY 96 Funding: $120K **Total Project Funds:** $320K

The focus of this project is the examination of the role of yttrium and other alloying elements on the microstructure and oxidation performance of improved single crystal nickel-based superalloys for advanced turbine applications. Anticipated improvements from these new alloys include enhanced durability and performance at the high temperatures required to improve energy efficiency. Specific 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.

23. Title: New Thermoelectric Materials for Solid State Refrigeration

ID: ORL95-10

PI: Brian C. Sales
Solid State Division

Phone: 423 576-7646

Partner: Marlow Industries Inc.
Dallas, TX

FY 96 Funding: $ 265K **Total Project Funds:** $ 700K

The goal of this project is to develop new materials that will significantly improve the performance of thermoelectric devices for solid state refrigeration and air conditioning. Thermoelectric refrigerators involve no moving parts, use no greenhouse gases, and are extremely reliable. ORNL

will synthesize candidate thermoelectric materials along several paths including filled and unfilled materials with the skutterudite structure and unusual "kondo-like" alloys. Marlow Industries will participate in the materials selection process, provide expertise and technical guidance on thermoelectric materials and concepts, and fabricate thermoelectric refrigeration devices for more complete evaluation of promising materials.

INTELLIGENT PROCESSING/MANUFACTURING RESEARCH

Sensors, Instrumentation, and Processing

24. Title: Resonance Ionization Mass Spectrometry Applied to Semiconductor Manufacturing

ID: ANL94-43

PI: Wallis Calaway
Materials Science Division

Phone: 708 252-3586

Partner: Bell Laboratories
600 Mountain Ave.
Murray Hill, NJ

FY 96 Funding: $125K **Total Project Funds:** $220K

The semiconductor industry has special requirements for instrumentation to characterize semiconductor materials and devices before and during the fabrication of integrated circuits. ANL is working in collaboration with Lucent Technologies and Bell Laboratories to demonstrate the applicability of a new surface analysis technique for materials characterization in support of semiconductor manufacturing. Surface Analysis by Resonance Ionization of Sputtered Atoms (SARISA) is an instrument developed at ANL for the purpose of studying fundamental problems dealing with surfaces. The aim of this work is to develop procedures for SARISA-type instruments that (1) lead to unambiguous identification of trace impurity in commercially significant silicon wafers and (2) allow quantitative determinations of dopants and impurities at low concentrations. Semiconductor manufacturing is a multibillion dollar industry in the U.S. that has been under extreme competitive pressure from foreign manufacturers. This collaborative work will help integrate this new type of instrument into the suite of analytical techniques available to solve problems in semiconductor manufacturing. This in turn should lead to improved fabrication procedures and increased competitiveness in the international market place for U.S. semiconductor manufacturers.

25. Title: Process Control for Laser Beam Welding

ID: ANL94-68

PI: Keng Leong
Technology Development Division

Phone: 708 252-3254

Partner: Low Emission Partnership
AC Delco Systems, World Headquarters
Flint, MI

FY 96 Funding: $145K **Total Project Funds:** $460K

Process monitoring and control capabilities are inherent requirements in the manufacturing of quality parts and the minimization of scrap. Concomitant reduction in energy and pollution is also achieved with the reduction in materials usage. This project is to develop a process monitoring/control system for the laser beam welding of steel components used in the automobile industry. The weld monitor is based on an ANL invention of an innovative technique for weld monitoring. The objective is to develop a weld monitor that is simple, low cost and rugged, suited for the manufacturing environment. The work carried out resulted in the realization that improved laser beam delivery systems are necessary for optimal development of the laser based processing method.

26. Title: Wear and Corrosion Resistant Coatings for Plastics Exposed to Alcohol Fuel Environments

ID: ANL94-85

PI: Robert Erck
Environmental Technology Division

Phone: 708 252-4972

Partner: AC-Rochester
1300 N. Dort Highway
Flint, MI

FY 96 Funding: $243K **Total Project Funds:** $720K

Alternative alcohol fuels (M85, E85) are being encouraged for use in automotive engines. Alcohol-based fuels attack common polymers, used in fuel systems, causing depolymerization and swelling or increased susceptibility to wear. The goal of this project is to develop processing or coating methods for low-cost polymers to be used in place of high-cost polymers. In any type of manufacturing, industry prefers low-cost raw materials that can be easily made into the finished part, e.g., by rapid injection molding. The benefits to industry would be the ability to substitute inexpensive plastic parts for metal parts in fuel systems. This benefits DOE by making the use of renewable alcohol fuels more attractive to consumers

27. Title: A Microspectroscopy Facility for New Infrared Imaging Materials

ID: BNL94-60

PI: Gwyn Williams
National Synchrotron Light Source

Phone: 516 344-7529

Partner: Grumman Corporation
MS A01-26
Bethpage, NY

FY 96 Funding: $110K **Total Project Funds:** $300K

In this project, BNL is developing a custom synchrotron beamline facility for characterizing infrared sensor technology materials. New materials for high performance and/or low cost infrared imaging systems will be developed and tested. The testing involves infrared microspectroscopy using infrared synchrotron radiation as the source for the microscope. Synchrotron radiation is 1000 times brighter than conventional thermal infrared sources, making this a unique facility.

28. Title: Development of a 10-Bit 500 MSample/sec Waveform Digitizer

ID: BNL95-05

PI: Maged Atiya
Physics Division

Phone: 516 344-3067

Partner: LeCroy Research Systems
700 Chestnut Ridge Road
Chestnut Ridge, NY

FY 96 Funding: $283K **Total Project Funds:** $526K

The aim of this research collaboration is to marry technological advances in the area of analog-to-digital conversion, recently introduced by LeCroy Research Systems, (LRS) with the proven long term experience of BNL in high speed digital technology. LRS has been a leader in ultra-high speed test instruments for the past 10 years. The BNL group has built and operated (since 1988) one of the first high speed (8-bits 500-MSample), high density, fast read-out waveform digitizer systems. A cooperation between LRS and BNL will yield a superior system that can be made available, as a

standard industrial product, to all interested users. The technology of high speed analog-to-digital conversion (and the associated technology of digital-to-analog conversion) is at the heart of many of the current civilian-sector innovations such as high definition television, multi-media, cellular communication, and high speed networks. The U.S. has been an undisputed leader in this area, holding a dominant position in both R&D and manufacturing. While there is increasing competition from foreign sources at the low- end of performance, an emphasis on the high performance devices should help retain this leadership. DOE laboratories, such as BNL, as well as industrial partners such as LRS, have long been active in this technology. This activity has been largely used to support the construction of instrumentation for basic research. The transfer of this technology to the industrial sector would represent a logical, and beneficial, step in the evolution of this technology. Additionally, by embedding high speed analog-to-digital conversion technology in systems capable of interfacing to standard high-speed computer buses, the benefits of this technology transfer will reach further into the industrial sector.

29. Title: Development of an In-Situ Scanning Surface Profiler

ID: BNL95-07

PI: Peter Tackas
Instrumentation Division

Phone: 516 344-2824

Partner: Continental Optical Corporation
15 Power Drive
Hauppauge, NY

FY 96 Funding: $132K **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 the Advanced Photon Source at ANL and ELETTRA at Sincrotrone Trieste in Italy. The In Situ LTP will provide valuable information to SR beam line scientists to enable them to utilize the powerful x-ray beams in the most efficient manner.

30. Title: Ion Source and Beam Control Technologies for Lithography

ID: LBL95-16

PI: Ka-Ngo Leung
Accelerator and Fusion Division

Phone: 510 486-7918

Partner: Advanced Lithography Group
9160 Rumsey Road
Columbia, MD

FY 96 Funding: $298K **Total Project Funds:** $549K

The goal of this project is to develop technologies for a hydrogen or helium ion beam projection lithography machine. Hydrogen or helium ion beam projection lithography can be used in creating extremely small (< 0.18 μm) features in the next generation of integrated circuits. In order to maintain the chromatic aberrations below 25 nm, an ion source which delivers a beam with an energy spread of less than 3 eV is required. In the past two years, the Ion Beam Technology (IBT) Group at the LBNL has been collaborating with the Advanced Lithography Group (ALG) in developing an ion source that can meet this requirement. This project has met or exceeded project goals. Ion beams have been generated with the required beam current and axial energy spread below 2 eV by employing a multicusp ion source together with a magnetic filter system. During the early part of 1996, the Ion-Beam Technology Group had designed and fabricated a new ion source based on the experimental results. The new ion source has already been delivered to the Advanced Lithography Group..

31. Title: Prevention / Elimination of Metal-Water Explosions in Aluminum Casting Pits

ID: ORL92-05

PI: Rusi P. Taleyarkhan
Engineering Technology Division

Phone: 423-576-4735

Partner: Aluminum Association
Pittsburgh, PA

FY 96 Funding: $400K **Total Project Funds:** $440K

Metal-water or steam explosions in aluminum industry casting pits have caused numerous injuries or fatalities and significant damage or destruction of infrastructure over the past fifty years. Traditionally, industry has attempted to prevent explosions by using an empirically-based approach involving the coating of sensitive surfaces with materials like Tarset Standard (TS). Due to environmental concerns and other reasons, TS is being discontinued from production, leaving industry the task of evaluating and finding alternate materials. As part of this project with the Aluminum Association (AA), ORNL is investigating how steam explosions initiate over specific surfaces, and what other coatings and novel methods may be appropriate as alternatives to TS.

Work has been in progress for less than a year and has resulted in one patent disclosure filed with the US patent office that uses a non-condensable gas source such as air, nitrogen, etc. to prevent steam explosions at sensitive surfaces. This approach promises to be a significant and cost-effective solution for the prevention of steam explosions in casting pits. Work has also resulted in the design of an experiment that simulates, in a laboratory environment, the interaction of molten aluminum contacting various submerged surfaces.

32. Title: Semiconductor Defect Data Reduction

ID: ORL94-56a

PI: Kenneth W. Tobin
Instruments and Controls Division

Phone: 423-574-8521

Partner: SEMATECH
Austin, TX

FY 96 Funding: $175K **Total Project Funds:** $ 175K

Automation tools for semiconductor defect data analysis are becoming necessary as device density and wafer sizes continue to increase. These tools are needed to efficiently and robustly process the increasing amounts of data so as to quickly characterize manufacturing processes and accelerate yield learning. Through a partnership with SEMATECH, an image-based method of analyzing process signatures, called spatial signature analysis software tool (SSAtool), has been developed. It uses statistical and morphological image-processing methods to achieve an automated segmentation of signature events into high-level, process-oriented categories. Spatial signature analysis of electronic wafermap data has been shown to improve the diagnosis and efficient correction of yield limiting conditions that arise in semiconductor manufacturing. Release 1.0 of the SSAtool has been installed at SEMATECH and is now being licensed to the instrument supplier community to ensure commercialization and long-term code support. Several SEMATECH member companies have also installed this software directly in their own fabrication facilities.

33. Title: Ultra-Precision Automated Measurement for Manufacturing

ID: ORL95-08

PI: C. E. Thomas
Instruments and Controls Division

Phone: 423 574-1155

Partner: InterScience, Inc.
Troy, NY

FY 96 Funding: $139K **Total Project Funds:** $230K

The goal of this project is to demonstrate a new level of automated process control, non-contact measurement technology for the U.S. manufacturing sector. The immediate goal is proof of concept for intelligent automated electronic interferometry inspection of digital microchips with a resolution better than the lithographic mask resolution (e.g., a transverse resolution of 200 nanometers and a longitudinal resolution of 20 nanometers). This will allow automated 3-dimensional inspection of the chips between processing steps to ensure success of the processing at each step; immediately identify process failures; save time, money, and energy; and improve quality and yield by eliminating defective chips early in the processing. The intention is to provide a totally automated, rapid, on-line inspection capability to automatically detect and sort defective chips or call for human intervention. This technology can be extended to inspection and process control for all kinds of precision components, particularly for the automotive, electronics, and defense industries. Some examples of additional uses include: automated inspection of precision machined parts; automated inspection of heads and platters for hard disk drives (where some tolerances are starting to approach the sub-micron level); and automated non-contact inspection of aircraft wing sections and automotive body panels on a more macroscopic level.

34. Title: An Implantable Drill Bit Monitor for Use in Oilfield Drill Bits

ID: ORL95-13

PI: David E. Holcomb
Instrumentation and Controls Division

Phone: 423 576-7889

Partner: Hughes Christensen
The Woodlands, TX

Houston Applied Research Center
Houston, TX

FY 96 Funding: $302K **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. Hughes Christensen, a U.S. company and currently the largest worldwide supplier of roller cone drill bits, would like to ensure that its drill bits avoid catastrophic failures. 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 $1,000,000 per well (worst case $5,500,000). On an annual basis, industry costs for bit cone loss range from $30,000,000 to $60,000,000. To avoid these failures, bits are typically replaced with significant remaining life. The costs associated with replacing a single bit can exceed $100,000.

35. Title: High Sensitivity Electrospray Ion Source Development

ID: PNL94-15

PI: Richard Smith
Environmental and Molecular Sciences Division

Phone: 509 376-0723

Partner: Finnigan MAT
355 River Oaks Parkway
San Jose, CA

FY 96 Funding: $145K **Total Project Funds:** $495K

The purpose of this project is to improve the understanding, and the actual performance, of the transport and focusing of charged particles that are formed at atmospheric pressure through the interface into the high vacuum region of a mass spectrometer. This improved understanding is intended to lead to the development and commercialization of an improved electrospray ion source for use in conjunction with mass spectrometers. In the project, PNNL will have primary responsibility for research on the source design at higher pressures (>1 torr), while the industry partner will concentrate on source designs at lower pressures (<1 torr). In FY 1996 a totally new concept for ion focusing was developed that promises to greatly exceed programmatic goals. Implementation of this novel "ion funnel" approach is the focus of current efforts.

36. Title: Development of a Near-Field Optical Microscope and Spectrometer

ID: PNL94-20

PI: Sunney Xie
Environmental and Molecular Sciences Division

Phone: 509-375-6882

Partner: Digital Instruments, Inc.
520 E. Montecito Street
Santa Barbara, CA

FY 96 Funding: $240K **Total Project Funds:** $595K

The objective of this project is to exploit the capability of conducting molecular spectroscopy at the nanometer scale. This would make possible implementing the wealth of techniques of optical spectroscopy with an unprecedented spatial resolution, and provide information about molecular species and their chemical reactions not accessible with the scanning electron microscope, the scanning tunneling microscope or the atomic force microscope. The high time resolution afforded by optical measurements would allow the observations to be made on the time scale of molecular motions during a chemical reaction. The impact of the successful development of this technology on several areas of science and technology, biological applications in particular, could be substantial.

37. Title: Nondestructive Analysis of Heat Treated Metal Microstructures for Intelligent Process Control

ID: PNL94-34

PI: Morris Good
Automation and Measurement Sciences Department

Phone: 509 375-2529

Partner General Motors Corporation
3900 Holland Road
Saginaw, MI

FY 96 Funding: $303K **Total Project Funds:** $570K

This project will develop ultrasonic backscatter as a sensing technology to provide intelligent process control when heat treating steel parts. Expected benefits include (1) fuel savings in the process for

making heat-treated parts used in automobiles, (2) increased energy efficiency in manufacturing by reducing scrap production, and (3) enhanced industrial productivity by replacing inefficient destructive tests of metal parts with nondestructive tests. Reduction of fuel used in the heat-treating of automotive parts is expected since margins of safety account for current variations of heat treatment. Research will include signal processing to provide measurement localization on non-round items, algorithm development to provide an acceptable measurement accuracy for ultra-rough surfaces, quantification of surface hardness and hardness of the underlying core material, establishment of relations between measurement and microstructure, and pilot tests at an industrial site.

38. Title: Inductively Coupled Plasma-Ion Trap Mass Spectrometer Development

ID: PNL95-29

PI: David Koppenaal
Materials and Chemical Sciences Division

Phone: 509 376-0368

Partner: Finnigan Corporation
355 River Oaks Parkway
San Jose, CA

FY 96 Funding: $219K **Total Project Funds:** $385K

The purpose of this project is to develop a new approach to elemental mass spectrometry. The proposed approach will be based on a novel instrument design comprising an inductively coupled plasma (ICP) ionization source and an ion trap mass spectrometer (ITMS)/detector. The project will build upon PNNL research experience in plasma-source mass spectrometry (MS) and Finnigan Corporation's technical and manufacturing expertise in ion-trap MS. The proposed collaboration will provide the essential foundation for Finnigan Corporation to proceed toward commercial development of a plasma source ion trap (product code-named PSQ). If successful, the proposed instrument will provide enhanced performance, lower cost, and smaller instrument size. The project will also explore and open scientific application areas for the new product to assist in developing a technical basis and for the developed instrumentation.

Fabrication

39. Title: Development of Rapid Prototyping Technology

ID: ANL94-18

PI: William Ellingson
Energy Technology Division

Phone: 708 252-5068

Partner: Spectra Group, Ltd.
1722 Indian Wood Circle
Maumee, OH

FY 96 Funding: $280K **Total Project Funds:** $840K

The purpose of this project is to develop technology related to the rapidly developing field of rapid prototyping (RP), also called solid freeform fabrication (SFF). In this work we are focusing on two aspects of RP technology; these are direct fabrication of functional ceramics and reverse engineering. Manufacturing technology is a critical industry in the United States and advances in manufacturing technologies which help keep the U.S. economically competitive are critical. This project focuses on just these issues. High volume manufacturing methods such as injection molding requires that fast turnaround times be established so that design iterations can be quickly accomplished. The way to do this is by using RP technology. Ceramic materials are an enabling technology for many high wear rate applications in manufacturing. By using reverse engineering, using 3-dimensional x-ray imaging in this case, allows verification of the as produced parts from RP. Coupling these two developments together here at the ANL has provided a unique position. This work is part of a large DOE activity involved with intelligent manufacturing which support the U. S. competitiveness position

40. Title: Microfabrication of a Multi-Axis Micro-Accelerometer Using High Aspect Ratio Microfabrication (HARM) and Silicon Micromachining

ID: BNL94-02

PI: John Warren
Instrumentation

Phone: 516 344-4203

Partner: Loral Control Systems
Kennedy Drive
Archibald, PA

FY 96 Funding: $250K **Total Project Funds:** $600K

The goal of this project is to use microfabrication methods developed at 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 instrument package that has a volume of about 8 cubic inches. Loral's prototype consisted of a precision-machined cubical enclosure that contains 18 levitation coils and 36 capacitive sensors. The primary goal of this project is to use high aspect ratio microfabrication to bulk fabricate all of these components, thus eliminating all 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 commercial aviation, auto navigation, active automotive suspension system control, drill bit navigation, and airbag deployment. The high aspect ratio microfabrication process has many scientific applications and is currently being used in the Instrumentation Division at BNL to construct prototype position-sensitive X-ray detector arrays that have many applications in high energy physics.

41. Title: Development of an Aluminum Bridge Deck System

ID: ORL94-56b

PI: H. Wayne Hayden
Metals and Ceramics Division

Phone: 423 574-6936

Partner: Reynolds Metals Company
Richmond, VA

FY 96 Funding: $ 620K **Total Project Funds:** $ 800K

The purpose of this collaboration with Reynolds Metals Company, is to combine Reynolds's verification experience and the manufacturing expertise of ORNL to refine the aluminum bridge deck panel system for commercialization using aluminum multi-void extrusions joined together to make panel 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.

42. Title: Rapid Prototyping of Ceramics

ID: ORL94-95

PI: Robert J. Lauf
Metals and Ceramics Division

Phone: 423-574-5176

Partner: 3D Systems, Inc.
Valencia, CA

Conway
Charlotte, NC

Argonne National Laboratory
Argonne, IL

FY 96 Funding: $ 293K **Total Project Funds:** $ 634K

The goal of this collaborative program is to develop fundamental knowledge and apply that knowledge to the technology of rapid product realization for structural ceramic components. A major part of the effort is directed to modifying solid freeform fabrication techniques to produce sinterable ceramic green bodies rather than plastic models. The program also recognizes the crucial role of advanced computational techniques for creating and manipulating the large data files needed to adequately represent complex three-dimensional components with the necessary resolution.

43. Title: Novel Methods for Fabrication Cost Reduction of Pressure Infiltration Cast Metal Matrix Composite Components

ID: ORL95-01

PI: James G. Hansen
Engineering Technology Division

Phone: 423 241-2102

Partner: Metal Matrix Composite Castings, Inc.
Waltham, MA

FY 96 Funding: $255K **Total Project Funds:** $ 760K

The goal of this project is to develop pressure infiltration casting as a method to manufacture high

quality metal matrix composite castings at high production rates. The manufacturing demonstration component of the project is a lightweight (60% reduction or 20 pound weight savings versus cast iron calipers), high modulus, particulate reinforced aluminum brake caliper for the Lincoln Town Car.

44. Title: Polymer Multilayer (PML) Film Applications in Optics, Electrolytes, and Glazings

ID: PNL94-06

PI: John Affinito
Materials and Chemical Sciences Division

Phone: 509 375-6942

Partner: E.I. du Pont de Nemours and Company
107 Market Street
Wilmington, DE

Sigma Labs
10960 Stallard Okace
Tucson, AZ

FY 96 Funding: $291K **Total Project Funds:** $716K

The purpose of this research collaboration is to apply the polymer multilayer (PML) deposition technology to a variety of commercial applications. The PML deposition technology utilized in the project is believed to offer substantial manufacturing advantages compared to current technology. Successful results in the project could enable the commercial use of several different types of new coatings that are currently not widely used due to a lack of suitable deposition technology. In the project, the industry partners will supply coatings materials for PNNL to apply in commercial applications selected by the industry partners. PNNL will develop and demonstrate the PML deposition technology in these commercial applications. The industry partners will carry out performance and environmental tests of the PNNL produced materials. For each product area, a database will be developed to determine which materials process parameters optimize the PML technique for each application.

45. 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
7201 Hamilton Boulevard
Allentown, PA

FY 96 Funding: $180K **Total Project Funds:** $730K

The purpose of this project is to develop tape calendering technology to produce mixed conducting, and oxygen ionically conducting, oxide membranes for use as air separation and oxygen production devices, and to transfer that technology to Air Products. Tape calendering 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.

Modeling and Computing

46. Title: Modeling of Electromagnetic Edge Confinement for Twin-Roll Casting

ID: ANL94-08

PI: John Hull
Energy Technology Division

Phone: 708 252-8580

Partner: Inland Steel
3001 E. Columbus Drive
E. Chicago, IN

FY 96 Funding: $120K **Total Project Funds:** $300K

The objective of this research is development of a computer model that can shorten casting research involving the use of electromagnetic fields for liquid-metal containment, stirring, and control. The model can also optimize the existing processes and minimize expensive, time-consuming, full-scale testing. The model can serve as a tool to assist U.S. manufacturers in the development and refinement of casting process and in the enhancement of the competitiveness of U.S. steel company in the world market.

47. Title: Application of High Performance Computing to Automotive Design and Manufacturing

ID: ANL94-54

PI: David Weber
Reactor Engineering Division

Phone: 708 252-8175

Partner: SCAAP Consortium
Dearborn, MI

FY 96 Funding: $437K **Total Project Funds:** $1,375K

Through collaboration, ANL, four other DOE national laboratories and the "Big Three" automakers (GM, Ford, and Chrysler) are developing high-performance computer systems that will "leapfrog" the technology automakers now use. This collaboration--the Supercomputer Automotive Applications Partnership (SCAAP)--is the 12th major R&D consortium formed under the auspices of the U.S. Council for Automotive Research (USCAR). ANL researchers are participating in the development of comprehensive numerical models for combustion, sprays, and aerodynamics in the design process. Specific partnership tasks include modeling in-cylinder fluid dynamics and conducting analyses of

vehicle aerodynamics; under-hood cooling; and heating, ventilation, and air-conditioning (HVAC) systems. ANL has focused on model development for HVAC and under-hood cooling analyses. In other areas partnership engineers are also developing efficient computational models of lightweight fiberglass composites, which automakers can use to design and manufacture lighter, crashworthy vehicles economically. Specific partnership tasks include developing new material and element models for composites, verifying and validating the models, and performing crash simulations on advanced computing architectures. The computational mechanics researchers at ANL are developing advanced element technology for use in large numerical (finite element) simulation of an all composite front structure during a crash process.

48. Title: Advanced Nuclear Power Plant Simulation

ID: ANL95-03

PI: David Weber
Reactor Engineering Division

Phone: 708 252-8175

Partner: Fauske and Associates, Inc.
16 W070 West 83rd Street
Burr Ridge, IL

FY 96 Funding: $233K **Total Project Funds:** $650K

This project is to develop an advanced nuclear power plant simulation capability. Nuclear power plants are complex engineering systems that are designed to operate safely, and the plant operators undergo extensive training for normal and off-normal conditions. The industry makes extensive use of computer-based simulators in training. The purpose of this CRADA is to develop an advanced power plant simulation computer code that will aid and train the plant operator in off-normal and accident conditions. The effort will take the present serial version, 4.0, of the Electric Power Research Institute (EPRI) code Modular Accident Analysis Program (MAAP) and create a new parallel software package by parallelizing the "driver" software and as many of the subroutine modules as possible. Further, additional phenomenological and system simulation capability will be added to the software. The software will be marketed by Fauske to the utility industry.

49. Title: A Regional High Speed Network

ID: BNL94-40

PI: Ted Daniels
Computing and Communications Division

Phone: 516 344-3237

Partner: NYSERNET, Inc.
200 Elwood Davis Rd.
Liverpool, NY

FY 96 Funding: $122K **Total Project Funds:** $200K

The object of this work is to develop a robust ATM based high-speed regional network suitable for early connection to the national information superhighway. It will assist NYSERNET in developing a standard ATM offering and provide a stimulus to common carriers to offer services in this area earlier than might have been possible without this project. The facilitation of ATM enabled applications in the areas of medical imaging, distance learning, desktop video- conferencing and computer visualization will benefit a number of DOE funded programs at BNL and in the wider DOE community

50. Title: Neural Network Model for the Sheet Metal Forming Die Design Process

ID: ORL95-90

PI: Gerald M. Ludtka
Metals and Ceramics Division

Phone: 423 574-5098

Partner: Lear
Morristown, TN

FY 96 Funding: $ 398K **Total Project Funds:** $ 905K

The goal of this project is to significantly reduce the required number of iterations in the sheet metal forming die design process, a process typically involving extensive and costly physical prototyping. The project employs a collection of emerging computational technologies such as digital simulations of deformation processes, neural networks, high-performance computing, and 3-dimensional optical metrology in order to achieve accurate and timely computations during the design process as well as during the control of the stamping process so as to eliminate a large fraction of the presently required design iterations.

51. Title: Modeling and Simulation of Advanced Sheet Metal Forming

ID: PNL94-38

PI: Mark Smith
Materials and Chemical Sciences Division

Phone: 509 376-2847

Partner: General Motors Research and Development Center
30500 Mound Road
Warren, MI

FY 96 Funding: $676K **Total Project Funds:** $1,370K

This project will enhance numerical modeling and simulation of advanced sheet metal forming processes, allowing rapid elevated temperature processing of lightweight aluminum alloy sheet. In this project, improved material deformation models and predictive codes for advanced forming processes will be developed. Development of the new capabilities will allow the manufacturing industries to optimize their component and tooling designs and improve the forming processes without costly trial and error development of the advanced forming technology.

SUSTAINABLE ENVIRONMENTS

Energy Conversion and Storage

52. Title: Lumeloid, A New Solar Energy Conversion Material

ID: ANL94-42

PI: Michael Wasielewski
Chemistry Division

Phone: 708 252-3538

Partner: Advanced Research Development, Inc.
359R Main St.
Athol, MA

FY 96 Funding: $302K **Total Project Funds:** $900K

The ANL is carrying out a research project in conjunction with Advanced Research Development, Inc. (ARDI) to develop photoactive polymer composite materials to directly convert solar energy into electricity. This technology utilizes ANL expertise in developing photoactive materials in combination with ARDI film technology to generate new material composites that could have a significant impact on cheap and efficient power generation from solar energy.

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

ID: BNL95-09

PI: Devinder Mahajan
Applied Science Division

Phone: 516 344-4985

Partner: Amoco Corporation
P.O. Box 3011
Naperville, IL

FY 96 Funding: $265K **Total Project Funds:** $726K

Natural gas conversion into liquid fuels is a viable option to transport remote gas. Methanol synthesis from synthesis gas, produced by partial oxidation of natural gas, can be catalyzed at a lower temperature (<150 C°) with a nickel complex in a homogeneous liquid phase that results in high methanolselectivity and high productivity. To utilize novel features of this "Liquid Phase Low Temperature Catalyst" and to develop a simplified and economical methanol synthesis scheme is the basis of the above referenced BNL/Amoco CRADA. A successful execution of this project is of obvious interest to Amoco. Development of an energy efficient process from a non-petroleum feedstock that addresses environmental issues, national security, and U.S. industrial competitiveness are some of the benefits tied to the DOE missions.

54. Title: Thin Film Lithium Batteries

ID: BNL95-11

PI: James McBreen
Applied Science Division

Phone: 516 344-4513

Partner: Power Conversion, Inc.
495 Boulevard
Elmwood Park, NJ

FY 96 Funding: $160K **Total Project Funds:** $531K

The BNL/Power Conversion, Inc. (PCI) project is focused on the development and testing of polymer electrolytes for primary thin film lithium batteries. PCI has developed a cell design, based on thin electrodes, with the cell enclosed in a thin heat sealed foil-laminate pouch like that used in the food industry (e.g. coffee). While this design is attractive for thin film batteries, and is adequate for prevention of ingress of water vapor or air, it presents many technical challenges. The foil laminate gives no mechanical support to ensure intimate contact between the electrodes and the electrolyte. Bulging of the pouch and its contents can result in large increases in the resistance losses in the cell. These problems were solved by the development of a new low cost polymer electrolyte, with good conductivity, and excellent adhesion to the electrodes.

55. Title: New Catalysts for Direct Methanol Oxidation Fuel Cells

ID: BNL95-14

PI: Radoslav Adzic
Applied Science Division

PI Phone: 516 344-4522

Partner: International Fuel Cells Corporation
195 Governors Highway
Windsor, CT

FY 96 Funding: $185K **Total Project Funds:** $510K

The goal of this project is the synthesis and characterization of a new efficient electrocatalyst for direct methanol oxidation fuel cells and development of a basic technology for catalyst fabrication. This will assist International Fuel Cells Corporation (IFCC) in their efforts to develop an efficient direct methanol oxidation fuel cell for electric vehicles. The catalyst should be compatible with the existing technology for the production of fuel cell electrodes. BNL is investigating a new approach for the catalyst design using metal oxides, perovskites, spinels, scheelites, or pyrochlores, as a support for a metallic Pt catalyst. These bifunctional catalysts should facilitate fast methanol adsorption and oxidation and concurrent fast oxidation of CO. Carbon monoxide, an intermediate in methanol oxidation, is the major poisoning species in this reaction and is the main obstacle for producing an efficient direct methanol oxidation fuel cell. The National Synchrotron Light Source (NSLS) at BNL and a variety of electrochemical and surface science techniques will be used to characterize and test the catalysts. The information obtained will help to improve the design of the new catalyst. Large scale testing of the catalyst will be performed with large area anodes and a 300 W, 5000 KWh direct methanol oxidation model fuel cell will be fabricated. Progress has been achieved in searching for active metal oxide-metal electrocatalysts for methanol oxidation with platinum electrocatalysts supported on several types of metal oxides. Synthesis and the electrochemical and/or spectroscopic characterizations were carried out. A very active electrocatalyst was obtained with Pt supported on Ru oxide. Reaction intermediates and products for some systems were characterized by in situ Fast Transform Infrared Spectroscopy (FTIR). The electrocatalyst supplied by IFCC has been characterized by electrochemical methods and Extended X-ray Absorption Fine Structure Spectroscopy (EXAFSS) and its activity compared with the best metal oxide-metal electrocatalyst synthesized at BNL.

56. Title: Rechargeable Zinc/Air Batteries for Consumer Applications

ID: LBL94-43

PI: Elton Cairns
Energy and Environment Division

Phone: 510 486-5028

Partner: Rayovac

601 Rayovac Drive
Madison, WI

FY 96 Funding: $124K **Total Project Funds:** $285K

The Zn/air battery is an especially appealing technology for use in consumer batteries because of its high specific energy, low cost and environmentally benign components. The zinc-air technology is greatly under-utilized because of the generally low power available from the cell. The power limitations stem primarily from the air electrode as a result of the slow kinetics of the electrochemical reduction of oxygen from air. Complete utilization of the zinc loading can also be a problem at high power drains. The focus of the project between Rayovac and LBNL has been to address these two limitations in order to extend the possible markets for the zinc/air primary battery technology. The first part of this project has been concerned with the application of novel electrocatalysts to the air electrode structure to improve the high-power performance of this electrode. The second part will focus on the study and modification of the zinc electrode formulation in order to optimize zinc utilization at high power. Four electrocatalyst systems are under study at LBNL. The electrocatalysts are added to the state-of-the-art Rayovac air electrode and performance is evaluated in the three-electrode configuration in the absence of zinc. Two candidates appear promising and will be delivered to Rayovac for incorporation into full zinc-air cells for testing.

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

ID: LBL95-27

PI: Frank McLarnon
Energy Conversion and Storage Division

Phone: 510 486-4636

Partner: Energy Research Corporation
Danbury, CT

FY 96 Funding: $110K **Total Project Funds:** $260K

In this project, Energy Research Corporation (ERC) and the LBNL are collaborating 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. 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. Together ERC and LBNL are working on additional improvements to lower the battery mass and to increase the ability of the electrolyte to wet the electrodes. To achieve these goals we are 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.

58. Title: Development of a Thin-Film Battery Powered Hazard Card and Other Microelectronic Devices

ID: ORL94-39

PI: John B. Bates
Solid State Division

Phone: 423 574-6280

Partner: Research International
Woodinville, WA

FY 96 Funding: $328K **Total Project Funds:** $470K

The goals of this research project are to investigate the feasibility of powering integrated circuit chips and compact microelectronic-based devices with thin-film, rechargeable batteries that can withstand temperatures of up to 200 C, and to determine and eliminate obstacles to their manufacturability. Since they have high energies per unit of volume and mass and because they are rechargeable, thin film lithium batteries have potentially many applications as small power supplies in consumer and medical microelectronic products. This research into battery technology will also enable the reduction in size and improvement in performance of existing microelectronic devices

59. Title: Development of a Thin Film Battery Powered Transdermal Medical Device

ID: ORL95-11

PI: John B. Bates
Solid State Division

Phone: 423 574-6280

Partner: Teledyne Electronic Technologies
Los Angeles, CA

FY 96 Funding: $313K **Total Project Funds:** $ 670K

Heart and brain activity are monitored by measuring microvolt signals developed on the surface of

the skin. Existing electrocardiogram (ECG) and electroencephalogram (EEG) recording units measure these small signals using electrodes attached to the skin. The objective of this project is to develop a thin-film battery powered preamplifier that would attach directly to the transdermal electrodes so that the small EKG and ECG signals can be amplified before transmission to the recording unit. These "active" electrodes will eliminate the effect of interference from ac pickup in the long cables from the recording unit and improve the reliability in diagnosing heart or brain malfunctions. By incorporating batteries into the circuit to power the amplifiers, no change to existing EKG or ECG recording equipment is required. The advantage of using the thin film solid state rechargeable lithium batteries developed at ORNL is that the active electrodes can remain as small as possible.

Energy Technologies

60. Title: Scale and Corrosion Inhibition in Boilers and Cooling Water Systems

ID: ANL94-23

PI: Carlos Melendres
Materials Science and Chemical Technology Division

Phone: 708 252-4346

Partner: NALCO Chemicals
1 Nalco Center
Naperville, IL

FY 96 Funding: $315K **Total Project Funds:** $870K

This research collaboration aims to develop a good understanding of the mechanism of scale formation in industrial boilers and cooling water systems and to formulate practical solutions to alleviate the problem. ANL technical expertise in aqueous corrosion research using spectroscopic and electrochemical techniques is being used in combination with NALCO's extensive experience in the synthesis and testing of chemical additives. Improved energy efficiency in boilers, the mitigation of corrosion, and lower operating and maintenance costs are among the many benefits that can be expected to accrue from the successful implementation of this program. Results obtained so far have provided new insights into the mechanism of oxide deposition on heated surfaces, as well as the deposition of carbonate phases on cooling water systems. Chemical formulations to inhibit these processes are currently being tested.

61. Title: Experimental Evaluation of Atomizing Nozzles of Fluid Catalytic Crackings Units

ID: ANL95-09

PI: Rajesh Ahluwalia
Technology Development Division

Phone: 708 252-5979

Partner: Amoco Research Center
P.O. Box 3011
Naperville, IL

FY 96 Funding: $250K **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 are not available. This CRADA between ANL and a consortium of oil refiners and an FCC nozzle vendor will fill the gap in knowledge by characterizing the performance of commercial feed nozzles using state-of-the-art laser-optics instrumentation. The consortium consists of Amoco Oil Company, Chevron Research and Technology Company, Phillips Petroleum Company and UOP. The performance data will allow the participants to select commercial nozzles that are optimal for their feeds and operating conditions. In a complementary task, a hydrodynamics model will be developed to determine the impact of atomization parameters on the overall yield of FCC units. The participants will use this information to design and fabricate advanced feed nozzles which will also be tested at ANL. This CRADA combines ANL's expertise in optical instrumentation and aerosol technology with participants' proprietary nozzle designs, field experience, and hardware. It supports DOEs missions of energy research and energy conservation.

62. Title: Condensing Economizers for Improved Efficiency and Reduced Pollution

ID: BNL94-22

PI: Thomas Butcher
Applied Science Division

Phone: 516 344-7916

Partner: Babcock and Wilcox
20 S. Van Buren Ave.
Barberton, OH

FY 96 Funding: $299K **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_2 particulates, and air toxics. Configured for pollution control, these systems have been named Integrated Flue Gas Treatment Systems (IFGT). The main objective of this project is to develop IFGT technology to the point 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 IFGTi 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 SOx emissions. The target market includes existing gas, oil, coal, wood, and waste-fired plants ranging in size from light industrial to utility. Participants include BNL, Consolidated Edison Company of New York, Inc. (Con Edison) ,Babcock and Wilcox Co. (B&W), and Condensing Heat Exchanger Corporation (CHX). At BNL small-scale pilot research is being

done with an emphasis on mechanisms of particulate capture. B&W is doing larger scale, application specific pilot tests with an emphasis on SO_2 and air toxics capture. B&W is also actively marketing these systems both as simple economizers and as integrated pollution control systems. At Con Edison, a full scale, 30 MW demonstration/test program is in progress.

63. Title: Production of Non-toxic Environmentally Acceptable Inhibitors for Corrosion Prevention

ID: BNL95-12

PI: Hugh Isaacs
Applied Science Division

Phone: 516 344-4516

Partner: W.R. Grace and Co
Washington Research Center.
Columbia, MD

FY 96 Funding: $213K **Total Project Funds:** $636K

Many corrosion inhibitors now in use are environmentally unacceptable (e.g. zinc, phosphate) and proposed legislation will exclude their use. A major difficulty facing industry (today) is to obtain acceptable (and cost effective) replacements for those inhibitors. The objective of this project is to produce effective non-toxic corrosion inhibitors for ferrous metal systems, (based on hydroxycarboxylates), and determine the mechanisms by which corrosion inhibition occurs. Using new electrochemical techniques, a series of environmentally acceptable organic anodic and cathodic inhibitors will be tested and compared with known inhibitors. By comparing effectiveness, the selection and combination of inhibitors will be optimized.

64. Title: A High-Resolution Subsurface EM Imaging Tool

ID: LBL94-14

PI: Ki Lee
Earth Sciences Division

Phone: 510 486-7468

Partner: Atlas Wireline Services
P.O. Box 1407
Houston, TX

FY 96 Funding: $215K **Total Project Funds:** $545K

The goal of the project is to develop and apply a new survey method and instrumentation for high-resolution subsurface 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 LBNL. The theoretical basis of the wavefield transform has been known for sometime, 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. We have since focused our effort 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 AWS to bring 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.

65. Title: Development of Low NOx Natural Gas Furnaces and Boilers

ID: LBL94-45

PI: Robert Cheng
Energy and Environment Division

Phone: 510 486-5438

Partner: Teledyne-Laars
6000 Condor Drive
Moorpark, CA

FY 96 Funding: $145K **Total Project Funds:** $435K

The goal of this project with Teledyne Laars is to exploit LBNL's lean premixed research burner (patent pending) for low emission commercial water heaters. Lean premixed (excess air) flames burn at a low combustion temperature which reduces NOx emissions. The simplicity of the LBNL burner appeals to Teledyne Laars' design engineers yet its operating principle is radically different from its commercial counterparts. The cost-shared research enables LBNL scientists to offer their fundamental combustion knowledge to re-design the burners for practical use. The Teledyne Laars engineers in turn contribute practical skills to develop a new commercial product. To date, a compact burner has been designed to operate under the requirements of a typical Teledyne Laars product. Tests performed with a 13 kW (50,000 Btu/hr) Teledyne Laars Telstar Spa heater fitted with a WSB reduced NOx emissions by more than 20 times (from 90 PPM to 4 PPM) without sacrificing efficiency. The partners are using these test results to finalize the specifications of an appropriate prototype for product development.

66. Title: Catalytic Conversion of Chlorofluorocarbons Over Palladium-Carbon Catalysts

ID: LBL95-45

PI: Gabor Somorjai
Materials Sciences Division

Phone: 510 486-4831

Partner: DuPont Company
Experimental Station
Wilmington, DE

FY 96 Funding: $250K **Total Project Funds:** $714K

Chlorofluorocarbons must be replaced as refrigerants and chemicals because of their adverse health effects (ozone depletion and other effects). The hydrodechlorination (HDCl) of C2F4Cl2 is a technology that uses a palladium catalyst supported on carbon. This project investigates the structure and bonding of reactants and products on palladium crystal surfaces that are also used as model catalysts. The elementary steps of the reaction and its mechanism are explored this way. The causes of catalyst deactivation will be studied, along with the use of promoters to inhibit it. The roles of the carbon support and the palladium-carbon interface will be explored as they influence the catalytic reaction rate and selectivity.

67. Title: In-Line Sensors for Electrolytic Aluminium Cells

ID: ORL95-04

PI: Jack P. Young
Chemical and Analytical Sciences Division

Phone: 423 574-5221

Partner: Alumax Corporation
Ferndale, WA

Kaiser Aluminum and Chemical Company
Pleasanton, CA
Reynolds Metals Company
Muscle Shoals, AL

FY 96 Funding: $160K **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. Along with the development of these sensors, the basic chemistry of the melts will be studied to gain knowledge of speciation and effect of impurities on the process efficiency. A critical parallel study will be carried out to develop sheath materials that will have a useful lifetime (6 months) in cryolite melts. With such sheath materials, the long-term measurement of temperature by standard techniques can also be accomplished.

68. Title: Moving Advanced Desiccant Materials 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 96 Funding: $ 191K **Total Project Funds:** $ 640K

This project is focused on advancing desiccant-based systems for cooling buildings. These systems have the potential to be applied in almost any commercial or residential building. The technology has several advantages over CFC- or HCFC-based (chlorofluorocarbon or hydrofluorocarbon) vapor compression equipment: (1) indoor air quality can be significantly improved, (2). fluorocarbon refrigerants can be eliminated or reduced, (3) electric energy use and demand can be lowered, with associated reductions in carbon dioxide emissions, and (4) new desiccant materials advances can generate new U.S. products and export opportunities. The partnership will develop the "enabling technologies" that would permit wide spread field application and successful commercial development of non-CFC cooling systems, Emphasis will be placed on developing a more versatile modeling tool to allow simulation of systems under varying configurations and dissicant materials.

69. 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

Partner: Advanced Vehicle Systems, Inc.
Chattanooga, TN

Nartron Corporation
Reed City, MI

Chattanooga Area Regional Transit Authority
Chattanooga, TN

Electric Transit Vehicle Institute
Chattanooga, TN

FY 96 Funding: $284K **Total Project Funds:** $ 670K

The primary technical goal of this project is to develop a mobile air conditioning system for an electric bus that is so highly efficient that the need for existing on-board propane powered sources will be eliminated. 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, and mass and size of the compressor will be reduced by incorporating advanced electric machinery systems technology that is only available at ORNL. The advanced system will then be installed in an Advanced Vehicle System's (AVS) electric bus that will be operated by the Chattanooga Area Regional Transportation Authority (CARTA) with Electric Transit Vehicle Institute liaison in the summer of 1997.

Environmental Technologies

70. Title: Development of Environmentally Acceptable Microbial Corrosion Control Methods

ID: ANL94-25

PI: James Frank
Energy Systems Division

Phone: 708 252-7693

Partner: The Gas Company
Box 3249
Los Angeles, CA

FY 96 Funding: $372K **Total Project Funds:** $840K

The ANL research program in microbiologically influenced corrosion (MIC) is focused on reducing MIC under conditions present in industrial environments while reducing environmental exposure to toxic chemicals (biocides) and cost. Three major, but integrated approaches are being pursued: use of chemicals such as some amines to control microbial colonization of metal surfaces; use of on line monitoring methods to detect rapid sustained pitting corrosion to optimize treatments; and modification of metallurgies to obtain MIC resistance.

71. Title: Bioremediation of Contaminated Soils by Enhanced Plant Accumulation

ID: ANL95-06

PI: Ray Hinchman
Energy Systems Division

Phone: 708 252-3391

Partner: Applied Natural Sciences, Inc.
7355 Dixon Drive
Hamilton, OH

FY 96 Funding: $201K **Total Project Funds:** $600K

Phytoremediation, an emerging cleanup technology for contaminated soils, groundwater, and wastewater that is both low-tech and low-cost, is defined as the engineered use of green plants to

remove, contain, or render harmless such environmental contaminants as heavy metals, trace elements, organic compounds and radioactive compounds in soil or water. This project includes a greenhouse experiment on zinc uptake in hybrid poplar that was initiated in 1995. This experiment is being conducted to confirm and extend field data from Applied Natural Sciences, Inc. indicating high levels of zinc in leaves of hybrid poplar growing as a cleanup system at a site with zinc contamination in the root zone of some of the trees. Because the roots sequester most of the contaminant taken up in most plants, a major objective of this program is to determine the feasibility of root harvesting as a method to maximize the removal of contaminants from soils. Available techniques and equipment for harvesting plant roots, including young tree roots, are being evaluated and modified as necessary for use with Phytoremediation plants.

72. Title: Oxygen-Enrichment Technology for Locomotive Engines

ID: ANL95-10

PI: Raj Sekar
Energy Systems Division

Phone: 708 252-5101

Partner: Association of American Railroads
50 F Street, NW
Washington, D.C.

FY 96 Funding: $249K **Total Project Funds:** $850K

The railroad industry is facing strict exhaust emissions standards for diesel-electric locomotives. Emissions of smoke, particulates, oxides of nitrogen (NOx), and hydrocarbons will have to be reduced to extremely low levels, and the measures needed to achieve these reductions are likely to have economic and fuel consumption penalties. Oxygen enrichment of combustion air has been shown to be very effective in controlling all criteria pollutants except NOx. An after-treatment scheme using monatomic nitrogen will control NOx. This project focuses on technology to enable the industry to meet the emissions regulations in a cost-effective manner. The problems to be solved are the development of an oxygen-enrichment membrane and a pulsed spark device for generating monatomic nitrogen, and the integration of these devices in a locomotive engine. The final goal of this project is a demonstration of the technologies in an actual locomotive.

73. Title: Conversion of Asbestos-Containing Material into a Non-Regulated Material

ID: BNL94-75

PI: Leon Petrakis
Applied Science Division

Phone: 516 344-3037

Partner: W.R. Grace and Co.
7379 Route 32
Columbia, MD

FY 96 Funding: $319K **Total Project Funds:** $470K

The purpose of this project is to develop a process for asbestos abatement in which the asbestos-containing material ("ACM") is sprayed with a chemical agent which converts the ACM into non-regulated material, after which the material can still function in accordance with its original purpose. Included is the development of a process for application of the conversion agent to the material in such a way that a negative-pressure enclosure will not be required.

74. Title: Biochemical Processing of Wastes Produced in Energy Production

ID: BNL95-02

PI: Eugene Premuzic
Applied Science Department

Phone: 516 344-2893

Partner: CET Environmental Services, Inc.
5845 Doyle Street
Emeryville, CA

FY 96 Funding: $108K **Total Project Funds:** $300K

Sludges generated during the production of electricity from geothermal resources typically contain hazardous waste concentrations of select heavy metals. In this project, a bioprocess for efficient removal of metals from sediments and sludges has recently been developed by the Applied Biochemistry Group in the Biosystems and Process Sciences Division (BPSD) at BNL. The toxic metals are converted to a soluble form, which allows their separation from solids. The technology is widely applicable and does not produce secondary waste streams. On a pilot scale, the process has been applied at BNL to geothermal sludges. The aqueous phase, which is generated in this process, can be reinjected into non-producing geothermal wells. CET Environmental Services, Inc. and Pacific Gas and Electric (PG&E) have an agreement allowing CET to use PG&E facilities, and site, to field test and develop the BNL technology under a CRADA between CET Environmental and BNL.

75. Title: A Pilot Scale Demonstration of Citric Acid Technology

ID: BNL95-13

PI: Arokiasamy Francis
Applied Science Department

Phone: 516 344-4534

Partner: Forrester Environmental Services, Inc.
38 Brookside Drive
Stratham, NH

FY 96 Funding: $160K **Total Project Funds:** $438K

In this project, toxic metals in bottom ash and fly ash from the incineration of municipal solid waste were extracted with citric acid followed by biodegradation of the citric acid- metal extract for metals recovery. In addition, methods for recovery of citric acid for recycling and precipitation of metals from citric acid ash extract were examined. The ash contained the following metals: Al, Ba, Ca, Cd, Cr, Cu, Mg, Mn, Ni, Pb and Zn. The extraction efficiency of the metals by citric acid was affected by the mineralogical association of the metals in the ash. The citric acid-metal extract was biodegraded by Pseudomonas fluorescens. The metals present in the extract were not toxic to the bacteria. During biodegradation of the citric acid extract, the metals precipitated from solution and were recovered along with the biomass. These results suggest the potential application of this technology to remove and recover the metal contaminants from incinerator ash and from other waste forms. After heavy metals extraction, the bottom ash should be more suitable for use in direct environment exposures such as road base and construction aggregates.

76. Title: Advanced Quadrupole Ion Trap Instrumentation for Low Level Vehicle Emissions Measurements

ID: ORL94-62

PI: Michelle V. Buchanan
Chemical and Analytical Sciences Division

Phone: 423 574-4868

Partner: Environmental Research Consortium
Dearborn, MI

FY 96 Funding: $304K **Total Project Funds:** $ 685K

Rapid, rugged, and cost-effective instrumentation for emissions monitoring is required both in the development of ultra-low emission vehicles and in meeting regulatory requirements. The primary goal of this collaboration is to develop an advanced quadrupole ion trap mass spectrometer (QIT) (a device for separating and sorting ionized molecules by their molecular weight) for the real-time measurement of trace components in automobile exhausts. This work should result in a "top 15" speciation analyzer and may provide the basis for fast oxygenated hydrocarbon and hydrocarbon analyzers and a methane/non-methane analyzer. The successful development of these devices will provide the U.S. automobile manufacturers with a competitive advantage over their non-domestic rivals in bringing ultra low emission vehicles (ULEVs) to market. This will also have obvious benefits to the air quality of our cities.

77. Title: An Exhaust Gas Flow Measurement System

ID: ORL94-71

PI: James E. Hardy
Instrumentation and Controls Division

Phone: 423-576-8670

Partner: Environmental Research Consortium
Highland Park, MI

FY 96 Funding: $192K **Total Project Funds:** $370K

The development of this state-of-the-art flow measuring system will enable the implementation of advanced and sophisticated vehicle emissions testing programs. These advanced testing programs are necessary to comply with new requirements of the EPA to measure extremely low concentration levels of emissions. The sophisticated analytical tools being developed depend on the capability to accurately measure the flow rate of the exhaust gas in real-time. While the near-term benefit of the technology developed under this CRADA is the ability to verify that vehicles meet new environmental regulations, the flowmeter will also be a tool used for vehicle development testing. The technology may also be applicable to DOE programs such as air quality monitoring.

78. Title: Development of Environmentally Conscious Machining Fluids

ID: ORL94-91

PI: Michael Sigman
Chemical and Analytical Sciences Division

Phone: 423-576-2173

Partner: Cincinnati Milacron
Cincinnati, OH

FY 96 Funding: $ 521K **Total Project Funds:** $ 895K

The objective of this project is to develop cutting fluids for ceramic and other advanced materials that are more environmentally benign and will reduce or eliminate the environmental problems associated with management and disposal of these cutting fluids. The specific goal of the project is to develop a method to degrade synthetic cutting fluids and reduce their total organic carbon (TOC) content and chemical oxygen demand to allow for final disposal in municipal sewage treatment facilities. Water-based industrial fluids can have excessively high TOC (ca. >15,000 PPM), thus making their treatment especially challenging.

79. Title: Hybrid Quantum Mechanical/Molecular Mechanical Methods for the Development of Pesticides, Dyes, and Polymers

ID: PNL94-10

PI: Mark Thompson
Environmental and Molecular Sciences Division

Phone: 509 375-6734

Partner: E.I. DuPont de Nemours & Company
P.O. Box 80328
Wilmington, DE

FY 96 Funding: $148K **Total Project Funds:** $367K

The purpose of this project is to apply Hybrid Quantum Mechanical/Molecular (QM/MM) methods to the development of pesticides, dyes, polymers , and general solution photochemistry. This project targets the chemical manufacturing industry's need to employ critical computational chemistry analytical tools. Pushing the state-of-the-art in application of these software tools is critical to both environmental compliance issues and the U.S. chemical industry's global competitiveness. Employing their extensive expertise in computational chemistry and chemical structure modeling, PNNL is collaborating with DuPont to perfect the parameterization of the QM/MM methods and development of leading edge analytical algorithms.

80. Title: Instrumentation for High Speed Analysis of Vehicle Emissions

ID: PNL94-12

PI: Jeffrey Griffin
Sensor Physics Group/Applied Physics Center

Phone: 509 375-2081

Partner: Environmental Research Consortium
330 Town Center Drive
Dearborn, MI

FY 96 Funding: $343K **Total Project Funds:** $1,010K

This project is focused on the development of new instrumentation and techniques to measure extremely low levels of vehicle emissions in an efficient and cost-effective manner. It is anticipated that vehicles of the future will need to meet emissions standards that are more rigorous than current levels. In order to verify that new vehicle technologies can achieve these levels, methods to rapidly measure low-level emissions are needed. This project is aimed at achieving this goal by: 1) developing a prototype instrument for rapid automotive emissions analysis that will identify and quantify all the major organic emissions components with a batch analysis cycle time of five minutes or less, and 2) design of a prototype instrument for rapid (one second time resolution) direct measurement of emissions' ozone-forming reactivity. Work conducted in this project will directly support efforts in a related cooperative program involving ERC, the Environmental Protection Agency, and the California Air Resources Board.

81. Title: Vehicle Exhaust Treatment Using Electrical Discharge and Materials Chemistry

ID: PNL95-10

PI: Thomas Orlando
Environmental and Molecular Sciences Division

Partner: USCAR
330 Town Center Drive
Dearborn, MI

FY 96 Funding: $210K **Total Project Funds:** $750K

This project will help determine the feasibility of plasma based technologies, using catalytic materials,

to mediate exhaust gas emissions from an internal combustion engine. The project is directed toward reducing the energy required to operate a plasma device and reducing both NOx emissions (especially under lean burn conditions) and hydrocarbons by the addition of catalytic materials. Work is focused on the development of a device and associate materials that will simultaneously oxidize hydrocarbons and reduce NOx. Technologies will be evaluated with regard to cold start and lean Nox applications with a goal of supplementing or replacing existing automobile catalytic converters.

82. Title: Supercritical Fluid Extraction Instrumentation and Methodology for Pesticide Residue Chemical Analysis

ID: PNL95-22

PI: Robert Wright
Materials and Chemical Sciences Division

Phone: 509 376-3002

Partner: DuPont Agricultural Products
P.O. Box 80402
Wilmington, DE

FY 96 Funding: $176K **Total Project Funds:** $650K

The ultimate objective of this project is to develop improved supercritical fluid extraction (SFE) instrumentation and methodology, demonstrate its practicality so that it can be routinely used during the crop protection chemical registration process, and transfer both the instrumentation technology and analytical-use methodology to appropriate industrial partners to allow the full advantages of the technology to be realized. Present sample preparation methods used in the routine chemical analysis of chemical residues from crop protection chemicals are time-consuming, use large quantities of organic solvents, generate hazardous waste, and generally offer relatively poor precision in the +/- 40% range. These factors contribute to the high cost associated with the registration of crop protection chemicals. Because of these high costs, the registration of minor use crops are in jeopardy; agricultural companies simply can not afford the cost, even when subsidized by the U.S. Department of Agriculture through the IR-4 program. SFE is a relatively new sample preparation technique that has the potential of revolutionizing current sample preparation methods used in residue and metabolism studies by greatly increasing the speed with which samples can be processed, reducing man-power requirements, significantly reducing the quantities of organic solvents and hazardous waste, and improving the quality of the resultant data. Feasibility studies have already been completed which demonstrate that SFE can efficiently remove crop protection chemical residues from soil and plant matrices.

83. Title: Solid Acid Environmental Catalysis

ID: PNL95-27

PI: John Nicholas
Environmental and Molecular Sciences Division

Phone: 509 375-6559

Partner: Catalytica
430 Ferguson Drive
Mt. View, CA

FY 96 Funding: $95K **Total Project Funds:** $396K

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. In collaboration with Catalytica Advanced Technologies of Mountain View, CA, (a small business) PNNL is working to understand the atomic-level details of catalysis, with the eventual goal of developing new catalysts that are environmentally benign. 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 Lab will be used to elucidate the fundamental aspects of catalysis, which are needed in order to develop new environmentally-benign products.

Biotechnology

84. Title: Rapid Prototyping for Bioceramics

ID: ANL95-08

PI: William Ellingson
Energy Technology Division

Phone: 708 252-5068

Partner: Zimmer, Inc.
P.O. Box 708
Warsaw, IN

FY 96 Funding: $136K **Total Project Funds:** $900K

The purpose of this project is to explore the extension of a DOE funded activity on a new manufacturing technology called rapid prototyping (RP) or solid freeform fabrication (SFF) to the rapidly accelerating cost area of medical technology. Specifically, this work focuses on studying the likelihood of economically extending rapid-prototyping and reverse engineering of ceramics to bio-ceramics, which can be used for orthopedic implants, bone-segment replacements, and other necessary skeletal applications. Small hand and arm-bone segment replacement, identified as having high workmen's compensation impact costs, are being explored for application of the technology. By using 3-Dimensional x-ray computed tomographic imaging data (reverse engineering) as a base for orthopaedic implant design, the replacement bone-segment or orthopaedic implant can be specifically designed for that patient. By using RP technology with developments that may allow tailoring the ceramic porosity structure near the surface, the time for complete bone engraftment would likely be reduced. This would significantly lower these costs and thereby reduce the overall medical community costs.

85. Title: Biochemical Production of Adsorbents from Fossil Fuel Wastes

ID: BNL94-49

PI: Mow Lin
Applied Science Division

Phone: 516 344-3064

Partner: EER Labs, Inc.
23778 Morslay Road
Altadena, CA

FY 96 Funding: $108K **Total Project Funds:** $235K

The production, transportation, and utilization of fossil fuels generates spent fossil fuel wastes. The fossil fuel wastes contain many of the EPA priority pollutants, such as polyaromatic hydrocarbons (PAH) and toxic metals. These wastes can be used as a feedstock in some biochemical processes which yield valuable products. The United States generates an annual amount of 1.2 billion gallons of used oil. About 200 million gallons of this oil is dumped at various municipal sites. To solve the waste oil problem, BNL and EER Laboratories have designed a preliminary plan for a 100,000 ton/year biomass production plant. The plant is designed for the utilization of less than 10% of the total waste oil dumped in the U.S. Even at this level, the economic studies have shown that the process is cost efficient, because it offsets the initial costs of waste disposal. Laboratory experiments for the production of biomass have been scaled up to 100 liter production capacity. In addition, several possible feedstock materials have been collected and tested for their suitability in the production of biomass. The feedstocks are waste oils collected from the New York and New Jersey area ranging from No. 2 fuel oil to No. 6 waste oils. Similarly representative samples of waste oils from California, e.g. KS-1 and KS-2 have also been secured. The produced biomass has been tested for its ability to adsorb heavy metals. The results were encouraging and indicate that the "biomass" may be used as an inexpensive ion-exchange material. The biomass is also being considered for further uses as protein feed and a source for the manufacture of lipids.

86. Title: DNA Repair Enzyme-Liposomes: Human Skin Cancer Prevention

ID: BNL95-03

PI: Betsy Sutherland
Biology Division

Phone: 516 344-3293

Partner: Applied Genetics, Inc.
205 Buffalo Ave.
Freeport, NY

FY 96 Funding: $272K **Total Project Funds:** $756K

Sunlight-induced skin cancer results from the induction of damage in DNA by UV in the solar spectrum, and from unsuccessful repair of that damage. AGI, Inc. has devised, and holds the U.S. patent on liposome products which deliver DNA repair enzymes to skin, thus increasing its ability to repair UV-induced lesions. As part of its program to test and validate the efficacy of these repair enzyme-containing liposomes, AGI wants to test their action at low levels of DNA damage which might be met in normal human exposure to sunlight. In this project, BNL has developed sensitive

methods for measuring DNA damage at low levels in non-radioactive DNA, including skin. The partnership of AGI and BNL will thus contribute to the development of methods for reduction of cancer, to new scientific knowledge and to the economy of the U.S.

87. Title: Instrumentation for High Throughput DNA Sequencing

ID: BNL95-06

PI: John Sutherland
Biology Division

Phone: 516 344-3279

Partner: LI-COR, Inc.
4421 Superior Street
Lincoln, NE

FY 96 Funding: $242K **Total Project Funds:** $282K

The objective of this project is to increase the number of DNA bases that can be determined in a single electrophoretic experiment. Such increases will decrease the cost per base of determining DNA sequence by reducing the number of times that an automated sequencer needs to be reloaded, a labor intensive, and hence expensive, process. Increasing read length in existing sequencers, such as the instrument marketed by LI-COR Corporation, will thus advance the goals of the human genome project and similar projects to sequence the DNA of organisms that are of commercial, agricultural, or medical interest. A major goal of this CRADA is determining electrophoretic conditions that will increase the length of read of the LI-COR sequencer without the need for extensive redesign and retooling. Central to this project is development of quantitative tools for objectively determining the performance of automated sequencers. Such tools are sadly lacking in the electrophoresis community, but without them, it is difficult to determine if changes in the configuration of an instrument result in meaningful improvements.

88. Title: Development of Proteins to Accelerate Tendon and Ligament Repair

ID: LBL92-08

PI: Richard Schwarz
Life Sciences Division

Phone: 510 486-4876

Partner: Amgen Corporation
1840 Dehavilland Drive
Thousand Oaks, CA

FY 96 Funding: $111K **Total Project Funds:** $275K

The goal is to develop a drug for improving tendon and ligament repair. This joint program will use technology developed at LBNL to produce and purify a biologically active factor. This technology will be combined with the expertise at Amgen to purify larger quantities, to micro sequence proteins, to clone and express genes. Tendon and ligaments repair very slowly in adults. The accepted view is that the endogenous calls respond poorly to the wounding stimulus and instead fibroblasts attracted to the wound site are recruited to accomplish the repair. One consequence is that wound repair is slow; another is that the newly deposited collagen fibers are not as aligned as in the original tissue and this results in healed area remaining structurally weaker than the original tissue. At LBNL, a major focus has been understanding gene regulation and how external signals influence the differentiated state of the cell. One cell system that has been extensively studied is embryonic avian tendon cells. This cooperative effort between LBNL and Amgen will not only speed progress but will take an important discovery past the point where it is only an intellectual curiosity to where its actual commercial potential is revealed.

89. Title: Neurochemical Imaging of Gene Therapy

ID: LBL94-09

PI: William Jagust
Life Sciences Division

Phone: 510 486-6241

Partner: Somatix Therapy Corporation
1301 Marina Village
Alameda, CA

FY 96 Funding: $357K **Total Project Funds:** $1,047K

Parkinson's disease is an extremely common neurodegenerative disease which results in loss of mobility, tremor, and eventually death. The disease is caused by a loss of dopamine-producing cells in the substantia nigra, and although some benefit is produced by treatment with L-DOPA, this treatment eventually fails in most patients. This project is designed to develop primate models of Parkinson's disease, and apply this model to a novel therapy of Parkinson's disease, using genetic engineering. The primate model used is MPTP-Parkinsonism, in which the neurotoxin MPTP is used

to destroy dopaminergic neurons, producing animals with Parkinsonism. PET scanning, using the tracer 6-[18F] Fluoro-L-m-tyrosine (FMT) is used to document and stage the severity of the dopaminergic lesion. Following this, animals are treated with genetically engineered fibroblasts which express one of several enzymes involved in dopamine synthesis, or with fibroblasts expressing brain trophic factors which produce neuronal growth and sprouting. PET studies with FMT are used to monitor the effects of these genetically engineered brain grafts to determine efficacy and time course of the therapeutic benefit.

90. Title: Cloning Genes for Diabetes

ID: LBL95-05

PI: Edward Rubin
Life Sciences Division

Phone: 510 486-5072

Partner: Rhone Poulenc-Rorer
500 Arcola Road
Collegeville PA

FY 96 Funding: $194K **Total Project Funds:** $583K

This collaboration with Rhone-Poulenc Rorer Inc. involves the use of transgenic mice to identify genes involved in atherosclerosis and its major predisposing conditions--diabetes and obesity. These studies utilize the unique ability to model genetically engineered mice after the human condition, and thus identify genes which contribute to the human condition. These studies are, in large part, dependent on the Rubin Laboratory's ability to create libraries of the human genome in transgenic mice. We have completed the creation of a 1.5 Mb in vivo library of chromosome 21 in a panel of transgenic mice. These animals have been analyzed with regard to distinct phenotypes associated with the presence of human DNA. We have been able to demonstrate specific developmental abnormalities in certain of these mice due to expression of the human DNA.

91. Title: Development and Commercialization of a Carbon Monoxide Occupational Dosimeter

ID: LBL95-30

PI: Gregory Traynor
Energy and Environment Division
Phone: 510 486-5729

Partner: Quantum Group, Inc.
11211 Sorrento Valley Road
San Diego, CA

FY 96 Funding: $100K **Total Project Funds:** $300K

In this project, Quantum Group, Inc. is working with the LBNL to develop an inexpensive passive carbon monoxide (CO) occupational dosimeter. CO is an unwanted by-product of energy production via fossil-fuel combustion and is one of the most deadly environmental pollutants encountered in indoor and occupational settings. Occupations such as forklift operators, automobile mechanics, bus drivers, toll booth operators, and parking garage attendants are all exposed to elevated levels of carbon monoxide. Many deaths occur every year from workers using gasoline-powered tools (e.g., cement cutters, power sprayers) in poorly-ventilated spaces. One obstacle in the way of identifying and mitigating high carbon monoxide environments is the lack of an inexpensive, passive, carbon monoxide dosimeter.

92. Title: Enzymatic Remediation of Waste Streams

ID: LBL95-37

PI: Alexander Glazer
Material Sciences Division

Phone: 510 642-3126

Partner: Enzymol International, Inc
Columbus, OH

FY 96 Funding: $112K **Total Project Funds:** $335K

This project is designed to develop the enzyme soybean peroxidase as a commercial product for the degradation of toxic waste chemicals such as polychlorobiphenyls (PCB's), nitroaromatics and, chlorophenols (CPC's). These highly toxic materials, of which several hundred million pounds have been released into the environment as a result of agricultural, industrial and munitions uses, are extremely persistent. Despite claims to the contrary, there is, at the present time, no generally applicable technology for their remediation. They resist bioremediation and give rise to other toxic compounds on incineration.

93. Title: Distributed Health Care Imaging on the National Information Infastructure (NII)

ID: LBL95-48

PI: William Johnston
Information and Computing Services Division

Phone: 510 486-5014

Partner: Kaiser Foundation
The Permanente Medical Group
Oakland, CA

FY 96 Funding: $200K **Total Project Funds:** $426K

The immediate goal of this project is the construction of a prototype environment that will allow access to high value, tertiary care health maintenance organization imaging facilities. Specifically, LBNL is developing a system in cooperation with Kaiser Permanente that will allow on-line access to coronary angiograms produced at Kaiser's San Francisco Medical Center Catheterization Laboratory. This Laboratory serves most of the Kaiser facilities in the greater San Francisco Bay Area, creating a typical problem in poor accessibility to records by physicians in the remote facilities. Health care information, especially high-volume image data used for diagnostic purposes (e.g. X-ray, CT, MRI, and cardio-angiography) are increasingly collected at tertiary (centralized) facilities. The importance of remote end-user access to these data is that the health care professionals at the referring facility (frequently remote from the tertiary imaging facility) will have ready access to not only the image analyst's (radiologist) reports, but the original image data itself.

94. Title: Structure of the Erythropoietin Receptor

ID: LBL95-49

PI: Thomas Earnest
Life Sciences Division

Phone: 510 486-4603

Partner: Amgen, Inc.
X-Ray Crystallography Lab
Thousand Oaks, CA

FY 96 Funding: $325K **Total Project Funds:** $844K

This project has a goal of determining the three-dimensional structure of the erythropoietin receptor (EPO-R) by x-ray and electron crystallographic methods. EPO-R is a transmembrane protein which binds to EPO (produced in the kidneys) and leads to the production of red blood cells, needed for oxygen transport. Recombinant human EPO-R is expressed in eukaryotic cells for purification, crystallization, and subsequent structure determination. Expression, purification, and crystallization of transmembrane proteins are all exceedingly difficult tasks compared to the case of water-soluble proteins, as is evidenced from the small numbers of structures of membrane proteins available. Once the structure is obtained, it will be analyzed to elucidate the structural mechanism of this signal transduction pathway, and to determine if small molecules can act as activators. EPO-R is homologous to a large number of other members of the cytosine receptor superfamily and thus can serve as a basis for attempts to understand the function of these molecules as well.

95. Title: Identification of Genes Affecting the Immune System, using Chromosomal Rearrangements in Mice

ID: ORL95-02

PI: Lisa J. Stubbs
Life Sciences Division

Phone: 423 574-0848

Partner: Darwin Molecular Corporation
Bothell, WA

FY 96 Funding: $220K **Total Project Funds:** $ 635K

The biotechnology segment of the pharmaceutical industry that utilizes cloned genes and advances in chemistry is rapidly emerging as an important producer of novel drugs, therapeutics, and diagnostics. Mouse mutations that are models of human diseases and are accessible to molecular cloning are invaluable raw materials in this industry. However, an important bottleneck has been the scarcity of clonable mouse mutations. To alleviate this problem, appropriate mutagenesis systems that are cloning-friendly and efficient schemes for identifying disease-producing mutations need to be developed. This collaborative project addresses this problem by exploring the utility of one class of mouse mutations - i.e., chromosomal rearrangements - for this purpose and screening for those that compromise the integrity of the animal's immune system. Most of these mutations have chromosomal exchanges in which the discrete breakpoints serve as starting points for molecular cloning, while a wide range of human disorders (such as cancer, diabetes, rheumatoid arthritis, and asthma) involve the immune system.

96. Title: Rapid Prototyping of Bioceramics for Implants

ID: ORL95-12

PI: April D. McMillan
Metals and Ceramics Division

Phone: 423-241-4554

Partner: Smith and Nephew Richards
Memphis, TN

FY 96 Funding: $ 190K **Total Project Funds:** $ 275K

The purpose of this work is to develop and commercialize net shape forming methods for directly creating dense Hydroxyapatite (HA) ceramic otologic implants. HA, in both dense and porous forms, is increasingly being used in bone replacement surgery because of its well established biocompatability. Otologic implants, because of their small size, are costly to manufacture by the traditional approach of machining from dense HA ceramic billets. ORNL's gelcasting process holds the potential of making these components by injection molding or other net-shape forming method. The technological hurdles that must be overcome to demonstrate gelcasting as a viable technique for this application include: development of biocompatible monomer / dispersant system suitable for HA powder; maintenance of dimensional tolerances in small components; and attainment of adequate green strength, green density, and economical process yields.

97. Title: Subsurface Microbial Culture Collection: Characterization and Screening

ID: PNL94-36

PI: F. Blaine Metting
Earth Systems Sciences Division

Phone: 509-372-0317

Partner: Zymogenetics, Inc.
4225 Roosevelt Way NE
Seattle, WA

FY 96 Funding: $76K **Total Project Funds:** $450K

The purpose of the project is to use molecular and physiological methods to characterize the DOE

Subsurface Microbial Culture Collection (SMCC) in order to identify the systematic relationships, metabolic diversity, and culturing requirements of individual strains so that subsets of strains can be screened using molecular, cellular, and whole animal protocols to reveal potential pharmacological activities. The pharmaceutical and biotechnology industries have traditionally screened microorganisms and other natural products for novel bioactivities leading to drug development. Recent scientific advances in molecular biology have resulted in new, highly specific methods for screening natural products for useful pharmacokinetic activities, thus significantly increasing the chances for identifying new drugs. The limitation to industry is access to novel genetic resources. Preliminary research suggests that the SMCC may be a unique genetic resource. The benefits to industry and society from the research would derive from the discovery of novel biological activity in one or more of the bacteria in the collection that could form the basis for development of a new drug(s). Targets for the proposed research include cancer, AIDS, diabetes, and other diseases.

Nuclear Medicine

98. Title: Medical Applications of Gadolinium- and/or Boron-labeled Pharmaceuticals

ID: BNL94-04

PI: Jeffrey Coderre
Medical Division

Phone: 516 344-2298

Partner: Boron Biologicals, Inc.
620 Hutton Street
Raleigh, NC

FY 96 Funding: $216K **Total Project Funds:** $600K

The purpose of this project is to identify new medical applications for a variety of newly synthesized boron-labeled compounds. We are currently screening a series of boron compounds to identify those with promising biological and pharmacological activities. From these we develop improved compounds for imaging and diagnosis of brain tumors using magnetic resonance imaging. MRI is a routine medical imaging procedure. Should the proposed gadolinium- labeled compounds prove to be more effective than the current generation of gadolinium-based MRI contrast agents, a major market would develop for U.S. pharmaceutical companies. Should any of the biologically active boron compounds prove to be useful for treatment of human disease states, a substantial market could develop for Boron Biologicals, Inc. (BBI). BBI is the only company in the world focusing on the R&D and manufacturing of biologically active boron compounds. As a small business, BBI has a very limited ability to test new compounds in biological systems. The Medical Department at BNL has an active research program in an experimental cancer therapy known as boron neutron capture

therapy (BNCT). BNL has the facilities and the expertise to evaluate new compounds in cell culture and in animal tumor models as well as the analytical instrumentation needed for quantification of low levels of boron in tissues or cells.

99. Title: A Specific Construct Approach to the Development of Peptide-Based Radiopharmaceuticals

ID: BNL94-61

PI: Prantika Som
Medical Division

Phone: 516 344-4239

Partner: RhoMed, Inc.
4216 Balloon Road.
Albuquerque, NM

FY 96 Funding: $329K **Total Project Funds:** $875K

The objectives of the project are to design, radiolabel, and evaluate synthetic peptides containing specific adhesive sequences for potential non-invasive clinical imaging of human pathological conditions. The receptor-binding peptides of adhesion molecules will be linked with an endogenous or synthesized radiometal-binding peptide sequence to construct a bifunctional peptide capable of binding 99mTc as a radioactive probe to target disease lesions, while still preserving the adhesive characteristics. The adhesive sequences are designed to target selected cell surface receptors and will be used for scintigraphic detection in animal models of experimental disease such as: a) thrombosis; b) non-neoplastic and neoplastic pulmonary disease; and c) inflammation. These synthetic peptides appear to be very promising for SPECT imaging in humans for the above disease conditions, and may overcome some of the problems encountered using monoclonal antibodies. The adhesion of blood elements to blood vessel walls and the underlying basement membrane is a dominant aspect of thrombosis, inflammation, tumor cell metastasis, and pathological tissue remodeling. Adhesion of platelets and lymphocytes, for example, is regulated by specific cell surface receptors found on a variety of molecules including those of the basement membrane and the activated endothelial cell surface. While adhesion molecules are generally quite large, the receptors on cells including those on platelets and lymphocytes can bind a number of short, specific peptide sequences derived from the parent adhesion molecule. The goal of this project is to link the receptor-binding peptides of adhesion molecules with an endogenous or synthesized radiometal-binding peptide sequence to construct a bifunctional peptide capable of binding 99mTc as a radioactive probe and to target disease lesions.

100. Title: A Radiopharmaceutical for the Treatment of Cancer-Related Bone Pain

ID: BNL95-01

PI: Suresh Srivastava
Medical Division

Phone: 516 344-4459

Partner: Diatide, Inc.
9 Delta Drive
Londonderry, NH

FY 96 Funding: $277K **Total Project Funds:** $770K

The goal of this project, in collaboration with the industrial partner, Diatide, Inc., is to develop tin-117m DTPA as a commercial radiopharmaceutical for the treatment of cancer-related bone pain. In approximately one-half million patients every year in the U.S. the cancer spreads to the bone. Most of these patients experience severe chronic pain which causes immobility and requires the use of major narcotic analgesics. In contrast to competitive technologies, Sn-117m DTPA provides substantial relief of bone pain without causing bone marrow toxicity or the adverse effects associated with the use of narcotic treatments. If successful in further clinical trials, tin-117m DTPA is expected to benefit this segment of patient population through the commercialization of this DOE/OHER supported technology by Diatide, Inc.

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

ID: BNL95-04

PI: David Schlyer
Chemistry Division

Phone: 516 344-4587

Partner: AccSys Technology Inc.
P.O. Box 5247
Pleasanton, CA

FY 96 Funding: $295K **Total Project Funds:** $813K

The purpose of this CRADA is to develop targets for the AccSys RFQ linac for the production of short-lived positron emitting isotopes for use in Positron Emission Tomography (PET). This accelerator could potentially be placed in a hospital in the Nuclear Medicine department as an aid to the wide variety of diagnostic procedures available with PET. These procedures might not be available otherwise since the half-lives of the radioisotopes used for PET range from 2 minutes to 2 hours and therefore have to be produced very near the location of their use. The attractive features of this accelerator are the relatively small size, the low cost and the low radiation field surrounding the accelerator during operation which makes it ideal for the hospital environment. The challenge of this accelerator is the development of reliable targets for producing the radioactivity which can withstand the high currents and pulsed nature of the beam.

102. Title: Medical Accelerator Technology

ID: LBL94-36

PI: William Chu
Accelerator and Fusion Division

Phone: 510 486-7735

Partner: General Atomics
3550 General Atomics Court
San Diego, CA

FY 96 Funding: $417K **Total Project Funds:** $1,500K

For more than four decades, under the auspices of DOE, LBNL pioneered and developed technologies of treating human cancer using accelerated heavy charged particle (proton and heavier ion) beams. In 1991 the first hospital-based medically dedicated proton accelerator facility was built in Southern California, and now the second hospital-based facility is being built in Boston by commercial firms. Although the first facility was build by a national laboratory, the second facility is being built as a turn-key system by the private sector, and the latter trend will continue. In this project, LBNL and the industry partner, General Atomics (GA) of San Diego, are cooperatively developing technologies to bring the extracted proton beam from the accelerator to the treatment room, and then channel it accurately into the treatment volume in a patient. Specifically, will be developed beam transport systems to bring the protons to the treatment rooms, a rotating gantry to aim the treatment beams precisely into patients from any angle, and patient positioners to align the patient accurately relative to the treatment beams. A patient treatment delivery system will be developed that controls the radiation dose in the patient, and hardware to improve the accelerator performances, including a radio frequency ion source and its low-energy beam transport system.

Advanced Computational Technology Initiative

103. Title: Development of a New Generation Framework for Parallel Reservoir Simulation

ID: ANL ACTI-95-95

PI: Tom Morgan
Mathematics and Computer Science Division

Phone: 630-252-5218

Partner: University of Texas (lead) ARCO, BP Exploration, Chevron, Conoco, Cray Research, IBM, Landmark Graphics (formerly Western Atlas Software), Mobil, Scientific Softwre-Intercomp, Schlumberger-GeoQuest, Texaco, and Unocal

FY 96 Funding: $167K **Total Project Funds:** $1,800K

The simulation of petroleum reservoirs is an important component in the development of more efficient techniques in petroleum recovery. Current simulators are fundamentally limited in the size and complexity of the problems that they can handle. Only through the use of parallel computing will the industry be able to tackle problems of current interest. This project provides the underlying R&D (the physics, mathematics, and computer science) required for the next generation of simulator codes. The purpose of the project is to provide a new-generation framework for petroleum reservoir simulation that (1) is suitable for high-resolution studies on massively parallel computers and clusters of heterogeneous workstations; (2) enables realistic modeling of complex physical processes including compositional, chemical, thermal, and coupled geomechanics; and (3) integrates subsurface and surface field management constraints.

104. Title: Subsalt Imaging with Marine Magnetotellurics

ID: LBL ACTI-95-90

PI: H. Frank Morrison
Earth Sciences Division

Phone: 510 486-5080

Partner: Scripps Institution of Oceanography, Amoco, BP, Chevron, Exxon, Geotools Corporation, NWG Associates, Texaco, Unocal, Conoco, and UC San Diego

FY 96 Funding: $203.8K **Total Project Funds:** $1,050K

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. LBNL is specifically assisting the 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.

105. Title: Subsidence, Analysis, and Control of Oil and Gas Reservoirs

ID: LBL ACTI-95-91

PI: Don Vasco
Earth Sciences Division

Phone: 510 486-5206

Partner: Long Beach Department of Oil Properties (LBDOP), Tidelands Oil Production Company (TOPKO), THUMS Long Beach Company, and California State Lands Commission

FY 96 Funding: $108.4K **Total Project Funds:** $225K

Subsidence is a drastic change in surface elevations usually caused when fliuds are extracted from the subsurface causing vertical shifts in the rock formations. The focus of this work is to develop computational tools to predict the surface subsidence associated with the development of oil and gas reservoirs. The approach is to couple a multiphase fluid flow simulation program to a routine for calculating surface displacements. The flow simulator chosen is the TOUGH2 package developed at LBNL. The pressure field produced by the TOUGH2 program is input into the surface displacement program. A simple homogeneous poroelastic half-space model was used to propagate the pressure changes to the surface. Testing was initiated for both a simple five-spot well pattern undergoing both water and steam flooding as well as a configuration of 46 wells conducting a waterflood patterned after the North Robertson field in Texas. The influence of reservoir heterogeneity on the calculated surface displacements was notable. LBNL scientists have completed coding and debugging a finite difference routine to compute surface displacements in an arbitrary three-dimensional poroelastic medium. The routine is quite efficient and may serve as a component of a planned inversion routine. LBNL is currently using the finite difference routine to predict surface displacements based upon volume injection data. Additional work has concentrated on incorporating the effects of temperature changes on surface displacements. For a steam flood, reservoir and overburden temperature may have an effect on surface displacements, in addition to reservoir

pressure, through the thermal expansivity of the poroelastic medium. This will allow reservoir simulations in which conductive heat transfer occurs from the reservoir to the overburden without requiring any more than the reservoir itself to be discretized. LBNL researchers are developing a code for determining variations in poroelastic parameters from volume injection and surface displacement measurements. This will allow researchers to calibrate the material properties using the waterflood data from the Wilmington field. Based on this approach investigators can then apply an existing inversion routine to determine volume changes in the reservoir from observed surface displacement data. In addition, the calibrated model, coupled with the reservoir simulator, may be used to predict surface displacement based upon various production scenarios.

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

ID: LBL ACTI-95-92

PI: Tadeusz W. Patzek
Earth Sciences Division

Phone: 510 486-5834

Partner: Cal Resources, Ltd., Mobil, Unocal, Crutcher Tufts, and Santa Fe Energy Resources

FY 96 Funding: $285.3K **Total Project Funds:** $750K

In oil fields with low-permeability reservoirs (diatomites, chalks, and carbonates), primary production yields only 2 to 6% of the oil-in-place. Fluids such as water, carbon dioxide, and steam are injected into reservoirs to increase or sustain oil production. The purpose of this project is to provide producers with an optimal injection policy that minimizes formation damage while maximizing oil production per unit volume of injectant. Injection can be very difficult to do properly. On one hand, injection rates must be low enough to prevent reservoir damage from overpressuring and inducing unwanted fractures. On the other hand, the rates must be high enough to make the costly operation viable. Historically, the conflict between prudent reservoir management and meeting secondary recovery targets has resulted in significant reservoir and well damage, injectant recirculation, and irreversibly lost oil production. In this project, LBNL is developing, with the help of a number of oil producers, an innovative Computer Assisted Operations (CAO) tool to promote better recovery from fractured, low-permeability diatomite reservoirs in Kern County, CA undergoing steam injection and water flooding. The tool functions by making "expert" decisions that balance fluid injection to maintain oil production versus the state of the reservoir; hence, prolonging production life by minimizing reservoir damage. Features of this project include: (1) real-time, well-by-well monitoring of the progress of injected fluid, along with the evolution of reservoir permeability and the fracture/matrix network; (2) neural networks for compiling individual well responses to injection, thus allowing predictive control; (3) reservoir simulation based upon trends recognized by the neural

network for making long-term injection policy decisions; and (4) project-wide coupling of well-head controllers that recognizes the oil field as a complex, coupled system. Feedback for global controller management comes from both the neural networks and reservoir simulation. This tool has been tested off-line, and LBNL is in the process of implementing it on-line at a selected part of the South Belridge field.

107. Title: Advanced Flux Visualization and Virtual Reality for Reservoir Engineering

ID: LBL ACTI-95-93

PI: Edward W. Bethel
Computing Sciences Division

Phone: 510 486-7353

Partner: Western Atlas Software (WALS)

FY 96 Funding: $99.2K **Total Project Funds:** $180K

Accurately determining the mechanisms of recovery in an oil or gas reservoir will directly affect the recovery efficiency of a given reservoir. A number of tools are used by engineers to understand the characteristics of these reservoirs with flux visualization a key parameter. Unfortunately, current technology limits the engineer's ability to easily interrupt the flux data. The objective of this project is to provide new computer visualization tools to enhance the ability of engineers to rapidly determine recovery mechanisms. A multidisciplinary team of computer and earth scientists at LBNL are exploring the use of advanced user visual interfaces, commonly called "Virtual Reality" (VR), coupled simulation, and modeling software. Working closely with industry, these efforts have resulted in an environment in which VR technology is coupled with existing visualization and computational tools. Two specific geoscience application areas are in development. In the first, LBNL scientists have developed VR technology to manipulate three-dimensional input parameters, such as the spatial location of injection or production wells in a reservoir simulator. In the second, scientists have demonstrated how VR technology can be used to manipulate visualization tools. Here the information is presented to the user in the form of a virtual injection well and is then applied to computing streamlines through fluxes. LBNL's project focus is on creation of a software infrastructure to support VR. This infrastructure is a collection of software "building blocks" and a visual programming interface for constructing a complete "program" for visualization. LBNL scientists can rapidly and easily interface several different VR input devices, such as a Spaceball or magnetic trackers, to a variety of computational or visualization tools.

108. 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

Partner: Meridian Oil, BP-America, and ARCO E&P Technology

FY 96 Funding: $498.2K **Total Project Funds:** $2,955K

The information available to the engineer on a drill rig platform is very limited 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. This project combines a unique mathematical modeling capability developed at 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. A three-year program is underway, bringing the technology to the point needed for commercialization. In this time period, development and testing will be completed for: graph-theory based computer models; well-site computer imaging and 3-D pore reconstruction techniques; a methodology for integration of model calculations with other direct and indirect measurements; and a methodology to ensure that results are representative of bulk rock behavior.

109. Title: Advanced Computational Tolls for 3-D Seismic Analysis

ID: ORL ACTI 95-09

PI: Jacob Barhen
Computer Science and Mathematics Division

Phone: 423 574-7131

Partner: Society of Exploration Geophysicists
Tulsa, OK

FY 96 Funding: $ 73K **Total Project Funds:** $ 400K

The development of a 3-D structural and stratigraphical model of hydrocarbon reservoirs is crucial for the future ability of the exploration industry to economically discover and produce oil and gas. It requires extensive use of 3-D seismic data. The global objective of this effort is to develop advanced computational tools for 3-D seismic analysis, and test the products using a model data set developed under the joint aegis of the United States Society of Exploration Geophysicists (SEG) and the European Association of Exploration Geophysicists (EAEG). These computational tasks are extremely expensive, and new ideas and methods are necessary to render them timely, efficient, and cost-effective. ORNL's aim is to develop leading edge U.S. capabilities in this application area of vital importance to the national economy by leapfrogging state-of-the-art seismic computation methods currently dominated by European technology. The availability of computer algorithms and software applications for exploiting the computational power and data-handling capabilities of parallel computers is essential to the routine adoption of 3-D seismic technology among oil companies. Demonstrating the effectiveness of the developed methods on the synthetic data sets produced by the SEG/EAEG 3-D Modeling Project will accelerate the adoption of the processing advances by the seismic industry. Additionally, the open publication of new methods tested on these models will assure their relevance as benchmarks, and an open discussion of the results obtained will assure a wide benefit to all companies.

ABSTRACTS OF SELECTED QUICK RESPONSE PROJECTS SUPPORTED IN FY 1996

Personnel Exchanges

110. Title: Exo-Melt(tm) Process

Oak Ridge National Laboratory
V. K. Sikka (423-574-5112)

Industrial Partner:
Philip Morris U.S.A:
S. C. Deevi (423-574-4352)

Total Project Funding: $35K

The objective of this completed personnel exchange project was to develop a commercially acceptable process for melting nickel and iron aluminides. The new process was required for two reasons: (1) The high-aluminum content of the aluminides does not readily permit the use of conventional melting methods, and (2) the exothermic nature of the formation of the compound from the constituent elements makes the melting process potentially unsafe. This project has developed a process known as Exo-Melt for the melting of nickel and iron aluminides. The process is based on a furnace-loading scheme that most effectively uses the heat of formation of the compound from its constituent elements. The process offers the following advantages: (1) 50% reduction in energy use, (2) 50% reduction in melting time, (3) inherently safe, (4) produces reproducible composition, (5) extends crucible life, and (6) save 50% of the cost. The Exo-Melt process has been extended from the development at ORNL to several melts at commercial vendors. In fact, the process has been licensed to United Defense/FMC (Anniston, Alabama) for the melting and casting of nickel-aluminide components. Since the signing of the license, 20,000 pounds of nickel aluminide have been melted and cast commercially. The Exo-Melt process won a R&D 100 Award in 1995 for outstanding technological innovation.

111. Title: Casting Process Simulator (CaPS)

Argonne National Laboratory
Richard Valentin (630) 252-4483

Industrial Partner:
Caterpillar, Inc.
Leo Chuzhoy (309) 578-6621

Total Project Funding: $75K

ANL and Caterpillar Inc. (Peoria, IL) have developed the Casting Process Simulator, or CaPS, for use in Caterpillar's foundry processes. Caterpillar used CaPS to perform more than 300 simulations of the casting process for more than 70 parts. By using CaPS, Caterpillar was able to improve its gating and risering systems. These improvements led to higher-quality castings with extremely low rejection rates. In addition to quality improvements, the new simulation program has provided environmental benefits as well. Using the new simulation, Caterpillar can achieve savings in raw materials used in the casting process. For example, each ton of iron cast, requires a ton of sand in the smelting process. A large part of this sand mixture becomes a waste product that is eventually sent to a landfill. Employing the CaP simulation in the casting process has improved yields by 100% and cut energy consumption and waste generation in half.

Small CRADAs

112. Title: Diffractive Null Compensators for Aspheric Testing

Oak Ridge National Laboratory:
Curt Maxey (423) 576-7114

Industrial Partner:
Diffraction International, Ltd.
S. M. Arnold (612) 945-9912

Total Project Funding: $68.5K

This project has achieved an order of magnitude reduction in the cost of testing aspheric optical components. The technology for testing aspheric optics using computer generated holograms (CGHs) as null lenses was successfully commercialized in a novel implementation compatible with commonly available optical test equipment. The product, the CGH Null Adapter, has commercially emerged with the enhancements provided through this project at a price that is affordable to the smallest optics manufacturers. The significance of this research collaboration extends beyond the technical and commercial benefits to the two partners (although Diffraction International now attributes over 50% of the its revenues to the CGH Null Adapter). Existing and emerging Department of Energy and ORNL programs (defense and manufacturing) that require precision aspheric optics now have access to the optical metrology technology and expertise for testing them with CGHs. The optics manufacturing community has responded eagerly to the opportunity to affordably implement aspheric testing with CGHs. The CGH Null Adapter has been nominated for multiple product awards and has attracted significant attention from a prominent optics magazine and a primary manufacturer of optical test instruments.

113. Title: Development of a Magneto-Optical Imaging System

Argonne National Laboratory
George Crabtree (630) 252-5509

Industrial Partner:
Phase Metrics, Inc.
Roger Taylor (619) 597-7955

Total Project Funding: $100K

Researchers at ANL and Phase Metrics (San Diego, CA) have developed a magneto-optical imaging capability called the Magnetic Flux Imaging System. This innovative device allows scientists to see for the first time the precise path of electrical current as it flows through high-temperature superconductors. The technique could be the key to developing superconducting materials that carry current 10 times greater than previously possible. The Magnetic Flux Imaging System won a 1996 R&D 100 Award and its developers won a 1997 Federal Laboratory Consortium award for excellence in technology transfer. Phase Metrics has used the new Magnetic Flux Imaging System commercially to evaluate high-temperature superconducting (HTS) thin-film devices. The system also has been used to analyze multifilament wires, as well as HTS materials used for magnetic levitation in flywheel energy storage systems being developed for utilities.

Technical Assistance

114. Title: Wetlands Characterization

Pacific Northwest National Laboratory
Dan Kaplan (509) 372-3004

Industrial Partner:
Soil Water Northwest
Richard Herriman (206) 338-5960

Total Project Funding: $4K

One area of significant concern and controversy for environmentalists and real estate developers is determining the exact boundaries of wetlands areas. This is more difficult than it appears to lay people, and is in fact a function of soil chemistry, not moisture content. Changing a wetlands boundary location by just a few feet can have large impact on project economics. Soil Water NW requested PNNL's technical assistance to develop a defensible technology for determining wetlands boundaries. In this project, PNNL invented a low-cost means that is objective and unambiguous. An invention disclosure was filed and PNNL is talking to potential partners about commercializing the technology.

115. Title: Tooth Contact Sensor

Pacific Northwest National Laboratory
Allen Lee (503) 417-7556

Industrial Partner:
TMJ Clinic
John Summer (503) 241-7353

Total Project Funding: $4K

Certain dental treatment protocols require a determination of the order, or sequence, of teeth contacts in the closing of the jaw. Present methods for this determination, including the use of carbon paper to mark points of contact, can be crude, making the extraction of timing information difficult. An alternative approach being developed by Dr. Summer uses the detection and timing of acoustic signals generated by the impact of the teeth. One technical difficulty preventing the implementation of this acoustic approach is the separation of the direct impact signals from the multiple reverberations from neighboring teeth. The PNNL developed and tested a unique transducer design and signal processing techniques which greatly improve the signal separation performance. Based on preliminary tests, the PNNL design and techniques promise to suppress extraneous signals from neighboring teeth and to provide unambiguous identification of the first tooth contact in a jaw closure.

APPENDIX A

CROSS REFERENCE TABLE FOR MULTI-YEAR PROJECTS*

	National Laboratory				
Program Focus Area	ANL	BNL	LBNL	ORNL	PNNL
Advanced Materials					
Synthesis and Processing	1, 2	3		4, 5, 6	7, 8, 9, 10
Materials Design and Characterization		11, 12, 13	14, 15, 16, 17	18, 19, 20, 21, 22, 23	
Intelligent Processing/ Manufacturing Research					
Sensors, Instrumentation, and Processing	24, 25, 26	27, 28, 29	30	31, 32, 33, 34	35, 36, 37, 38
Fabrication	39	40		41, 42, 43	44,45
Modeling and Computing	46, 47, 48	49		50	51
Sustainable Environments					
Energy Conversion and Storage	52	53, 54, 55	56, 57	58, 59	
Energy Technologies	60, 61	62, 63	64, 65, 66	67, 68, 69	
Environmental Technologies	70, 71, 72	73, 74, 75		76, 77, 78	79, 80, 81, 82, 83
Biotechnology	84	85, 86, 87	88, 89, 90, 91, 92, 93, 94	95, 96	97
Nuclear Medicine		98, 99, 100, 101	102		
Advanced Computational Technology Initiative	103		104, 105, 106, 107, 108	109	

* The numbers listed in this table refer to the project sequence numbers in this book.

APPENDIX B

ALPHABETICAL LIST OF INDUSTRIAL PARTNERS*

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

APPENDIX C

ALPHABETICAL LIST OF PRINCIPAL INVESTIGATORS*

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