FY 1992

Accomplishments

Office of Basic Energy Sciences

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Introduction

The Office of Basic Energy Sciences (BES) annually funds over 1,300 research projects at about 200 U.S. universities, DOE laboratories, and industrial institutions. The other major function of the BES program is the design, construction, and operation of complex scientific facilities for use by the research community to conduct experiments in basic research in areas which underpin the Department's energy objectives. These activities provide support for about 4,300 professors, post-doctoral fellows, and graduate students at universities and about 1,800 full-time senior scientists at DOE laboratories. The BES subprograms listed below support research in basic energy sciences that results in over 11,000 published reports of scientific findings in peer-reviewed journals annually.

The following selection of accomplishments for Fiscal Year 1992 does not reflect the full range of activities under the program. It does, however, provide examples of how basic research can contribute to solving a wide variety of energy problems. The accomplishments are presented in four sections:

The following subprograms were managed and/or funded under Basic Energy Sciences during Fiscal Year 1992.

Materials Sciences (MS)
Chemical Sciences (CS)
Engineering and Geosciences (EG)
Applied Mathematical Sciences (AMS)*
Energy Biosciences (EB)
Advanced Energy Projects (AEP)
Small Business Innovation Research (SBIR)**

* Managed by the Scientific Computing Staff of the Office of Energy Research; Accomplishments for AMS not included.
**Managed under Advanced Energy Projects.

Accomplishments

Major Facilities-Related Accomplishments

Advanced Light Source (ALS) Achieves Important Milestones

On January 29, 1992, at the Lawrence Berkeley Laboratory, electrons were accelerated in the ALS booster synchrotron to the full design energy of 1.5 GeV. Then, the first electron beam to be successfully extracted from the booster synchrotron occurred on March 20, 1992. Approximately 4 milliamperes of beam current, at an energy of 850 MeV, with a repetition rate of 1 hertz was extracted and transported into the Booster-to-Storage Ring Beam Transfer Line where it was then fed into a beam dump. This was an important step in the process leading to the storage of the electron beam in the ALS storage ring.

The Advanced Light Source (ALS) Receives Engineering Excellence and Design Excellence Awards

The 1992 American Consulting Engineers Council Honors Awards included the firm of Keller & Gannon for their work on the ALS at Lawrence Berkeley Laboratory. There were 141 finalists in the competition of which 24 were selected to receive special recognition at the national level. The awards were presented at the Hyatt Regency in Washington, D.C., on April 10, 1992.

The San Mateo County Chapter of the American Institute of Architects honored the winners of its 4th Biennial Design Awards on March 20, 1992. Reid & Tarics Associates of San Francisco won top honors with two Awards of Design Excellence. One of the Awards of Design Excellence was for the ALS.

New Opportunities Identified for Soft X-ray Wavelengths at the Advanced Light Source (ALS)

The rapidly approaching commissioning of the ALS at Lawrence Berkeley Laboratory (LBL) is awaited with much anticipation by researchers in the physical and life sciences because of the numerous research opportunities afforded by the machine. These opportunities have been summarized and discussed in an article by David Attwood, Director of the Center for X-Ray Optics at LBL, published in the August issue of Physics Today. Dr. Attwood reviews the capabilities of the ALS, experiments presently underway at existing synchrotron sources and how these combine to present new and challenging options, and opportunities for future research beginning early next year when ALS goes into operation.

Semiannual Construction Project Review Held at the Advanced Photon Source

On-site semiannual reviews of the Advanced Photon Source (APS) took place on April 27-29 and August 25, 1992. There was a schedule slippage in the utility building; however, the utilities needed for commissioning will be completed in time to meet the commissioning schedule. Construction at the site is moving well; the LINAC cave is ready for beneficial occupancy by the APS project. The Level 0 milestone, "Initiate Installation of the LINAC Technical Components" (baseline schedule April 30, 1992), was approved by the Deputy Secretary. Argonne National Laboratory has been authorized to initiate installation. The rest of the LINAC building will be finished by December 1992, in time to support the LINAC installation plan. Concrete work for the synchrotron building is complete, and the storage ring shield is beginning to take shape. A portion of the experimental half of the "Early Assembly Area" will be completed and made available for storage-ring assembly activities by January 1993. The review committee noted a considerable improvement in project management, particularly in the areas of scheduling and procurement. The project continues to maintain an outstanding record of construction safety. There have been only two lost-time accidents (back injuries) in 310,000 manhours with 130 days elapsed since the last accident. The project is scheduled for completion in the third quarter of 1996.

Meeting Held With the Materials Research Collaborative Access Team (MR-CAT)

Members of the Division of Materials Sciences met with four representatives of the MR-CAT (Bruce Bunker/University of Notre Dame, John Houston/Amoco Research, Steve Nagler/University of Florida, Pulak Dutta/Northwestern University) on May 4, 1992, to discuss funding for the MR-CAT beamline at the Advanced Photon Source (APS). The overall cost of the beamline is estimated to be about $8.6M (in addition to the front ends and insertion devices, valued at about $1.5M, provided through the APS project). Amoco has committed $1.7M; the States of Florida and Illinois will be asked to contribute $1.0M and $0.5M, respectively; the Universities of Florida and Notre Dame will provide $0.6M and $0.3M, respectively; and DOE/Basic Energy Sciences (BES)/Division of Materials Sciences (DMS) will be requested to provide about $2M, as will the National Science Foundation. The science to be done with this sophisticated instrumentation will be carried out on several experimental stations with radiation generated from a bending magnet source as well as a tapered undulator. The experimental techniques would include XAFS, reflectivity, diffraction, wide and small angle, X-ray scattering, time dependent X-ray scattering, magnetic X-ray scattering and diffraction anomalous fine structure. The scientific program would include: a) structural phase changes; b) disordered alloys and amorphous materials; c) growth and recrystallization, surfaces, and interfaces of electronic materials; d) catalysts; e) structure of confined liquids; f) polymers and organic thin films. It is likely that a proposal to DOE/DMS will be received requesting partial support for the construction of the instrumentation.

High Flux Isotope Reactor (HFIR) Passes Hydrostatic Proof Test; Resumes Iridium Production

The first Hydrostatic Proof Test of the HFIR reactor vessel at Oak Ridge National Laboratory since 1987 was successfully completed on March 5, 1992. The test demonstrated the integrity of the reactor vessel for an additional 10 operating years. However, the test is currently required by HFIR Technical Specifications to be performed for every year of operation.

Seventeen iridium targets have been loaded into the reactor to resume production of iridium-192. Prior to the extended reactor shutdown in 1986, HFIR was producing iridium-192, which is used extensively in commercial radiography.

Presently, this material is in great demand, and this effort is being strongly encouraged by the Office of Nuclear Energy. In the near term, iridium targets will be prepared for HFIR at the Advanced Test Reactor facility in Idaho where iridium-192 is also produced. The targets are placed in locations of the reactor which are not routinely needed for other research, thereby increasing the overall benefit of the reactor.

Stanford Synchrotron Radiation Laboratory (SSRL) Satisfies ES&H Requirements and Begins Operation

On February 12, 1992, the Stanford Synchrotron Radiation Laboratory was notified by the DOE San Francisco Field Office that it had satisfied ES&H requirements and received approval to operate the facility. SSRL successfully completed, over the last 6 months, three ES&H documents: (1) a response to the Tiger Team Assessment conducted last Fall; (2) an Accelerator Operational Readiness Review (AORR) associated with the construction of an electron injector completed in the Fall of 1990, since commissioned; and (3) certification that improvements made to the storage ring, SPEAR, are in compliance. At the time the AORR was conducted, an Accelerator Safety Order had yet to be issued and SSRL had to rely on adaptation of DOE Order 5480.5 written for safety of nuclear facilities. The AORR is the first conducted for an accelerator and the experience gained from the review assisted writing a new and more appropriate Accelerator Safety Order now in advanced draft. As a result of satisfying these requirements, SSRL was able to meet its schedule for a 7-month users run from February to September 1992. This run is the first since SSRL became independent of SLAC's LINAC electron source and the first since the upgrading of SPEAR. The users run accomplished 90% uptime and accommodated over 600 scientists conducting over 100 experiments on 20 beamlines.

Basic Energy Research Advances

Chemical Analysis of Single Red Blood Cell Now Possible

A Chemical Sciences investigator, Dr. Edward S. Yeung at Ames Laboratory, has developed a procedure for the analysis of the chemical contents of a single red blood cell. This biological sample is at least 50 times smaller than previous work. In Dr. Yeung's new technique, a single blood cell is introduced into a small capillary under a microscope, the cell is lysed by the buffer in the capillary and its contents analyzed using capillary zone electrophoresis. Laser excitation is used to detect fluorescence species (10^{-20} mole range ≈ 1000 molecules) and nonfluorescent species (10^{-17} mole range, ≈ 1 million molecules) are detected indirectly by a charge displacement mechanism. The detection scheme was based upon a design which won a 1991 R&D 100 Award.

Results for the single blood cell included the determination of the Na^+/K^+ ratio and the in vivo study of glutathione oxidation/reduction. The development of analytical techniques with these detection limits and sample volumes opens a new realm of biochemical analytical chemistry. Single cell analysis could be used for disease characterization before the gross manifestations of the disease becomes apparent. Similarly, drug studies could now be carried out at a single cell level rather than testing a living organism for the pharmacological effects of the test compound.

Experiment Confirms Prediction of Systems With Unusually High Hydrogen-Storage Capability

A surprising theoretical prediction that one positively-charged metal ion can bind as many as ten hydrogen molecules was made by Materials Sciences grantees, Professors P. Jena and B. K. Rao of the Virginia Commonwealth University. Details of their prediction were reported in an article published in the Physical Review Letters. This prediction received experimental confirmation in late May. Michael Bowers of the University of California - Santa Barbara observed the binding of up to seven H_2 molecules to a Co^+ ion. This was the first prediction of molecular chemisorption to a transition metal ion. The binding energies and equilibrium geometries of the H_2 molecules bound to the ion was calculated. The experimentally determined geometries and binding energies are also consistent with prediction.

This experimental verification is important in the search for environmentally safe storage of energy. The ability of the positively charged ion to trap a large number of hydrogen atoms has important implications in problems associated with hydrogen storage, since ions can be isolated in matrices such as zeolites, and can also be expected to have implications in the understanding of heterogeneous catalysis.

Biodegradable Plastic to be Harvested From Plants

A research study published in the April 24, 1992, issue of Science emanating from Michigan State University/DOE/Plant Research Laboratory effectively demonstrates that it is possible to transfer the genes from a bacterium into a higher plant and have them expressed in producing polyhydroxybutyrate, a polymer that can be made into a biodegradable plastic. While the results are only preliminary, with appropriate research and development in the future, such findings could well be used as the basis for entirely new biotechnological industries that would replace the use of fossil resources with renewable resources. This achievement received wide recognition in the general press, both in the U.S. and abroad.

Transition State Directly Observed for the First Time

The heat from combustion processes is derived from the breaking and making of chemical bonds. Understanding, characterizing, and predicting these processes are fundamental to designing new combustion devices to meet national energy and environmental goals. On the way from reactants to products, a chemical reaction passes through what chemists term a transition state. In this state, for a brief moment, the participants in the reaction look like one large molecule ready to fall apart. Though predicted theoretically for nearly 70 years, the transition state has eluded direct experimental observation and verification. However, in an article in the June 12 issue of Science, and highlighted on its cover, is just such an experimental observation by a group from Lawrence Berkeley Laboratory (LBL). The report describes how it is possible to directly probe the transition state and provide confirmatory evidence of the theory.

The thermal dissociation of a molecule, typically at high temperatures, is an example of a unimolecular dissociation. A quantitative description of the dissociation process was developed in the 1920's by Rice, Ramsberger and Kassel and later refined by Marcus. The RRKM theory has been difficult to verify experimentally, despite extensive efforts to do so, because experiments have lacked the energy resolution needed to resolve the structure of the transition state in the energy dependence of rate constants. RRKM theory predicts that the rate constant of a reaction will increase in steps, due to quantization in the transition state and the energetic accessibility of vibrational levels of the transition state, as the vibrational energy of the reactant is increased. In an experimental "tour de force," C. Brad Moore and his students at LBL have been able to measure the rates for the unimolecular dissociation of ketene using laser techniques with adequate resolution to resolve the vibrational levels of the transition state. The experiments show stepwise increases in dissociation rate as the internal energy of the reactant is increased, a result that is consistent with RRKM theory.

Elastic Properties of Cracked Solids Described in Major Review Article

A major review on "Effective Elastic Properties of Cracked Solids: Critical Review of Some Basic Concepts" by Professor Mark Kachanov of Tufts University was published in the August 1992 issue of Applied Mechanics Reviews (AMR). AMR provides an assessment of the world literature in engineering sciences on a monthly basis.

In the paper, various approaches to the problem of effective moduli of cracked solids are critically reviewed and are further assessed by comparing their predictions to results for sample deterministic arrays. It was found that the approximation of noninteracting cracks has a wider-than-expected range of applicability. Also in the spirit of "damage mechanics," it was argued that there is no direct quantitative correlation between progression of a microcracking solid toward fracture and deterioration of its stiffness; thus, the effective moduli may not always serve as a reliable indicator of damage.

Professor Kachanov is a principal investigator in the Engineering Research Program of the Division of Engineering and Geosciences.

First Relativistic Heavy Ion Atomic Collision Cross Section Measurement

The first cross section measurements of an atomic collision process involving relativistic heavy ion energy beams were completed by Oak Ridge National Laboratory scientists supported by the Chemical Sciences Division. The experiments were performed at a CERN accelerator and showed that collisions of Tev energy sulfur ions with heavy atom targets created a significant number of electron-positron pairs. The pairs were created, not by a direct collision, but by the Coulomb interaction that resulted in an energy-to-mass conversion. The cross sections obtained were found to be consistent with Quantum Electrodynamics Theory. The findings are important to establishing more appropriate operating parameters for heavy ion accelerators and to reduction of the interfering background in the next generation of heavy ion nuclear experiments.

Practical Correction Procedure Found for Inexpensive Solar Radiation Detectors

Quantitative evaluation of the solar energy potential of specific geographic sites and global change modeling require knowledge of time-averaged solar energy flux. Widespread measurement of solar irradiance has been precluded by the high capital and significant maintenance costs of first class thermopile instruments. In Solar Energy (47,#4, 1991), scientists from Pacific Northwest Laboratories (B. LeBaron) and the State

University of New York at Albany (J. Michalsky, R. Perez, and L. Harrison), supported by the Basic Energy Sciences Geoscience Program, describe a simple correction procedure for an inexpensive silicon cell-based solar irradiance detector. Application of this approach results in performance comparable to first class instruments at a significant reduction in cost, thereby enabling more extensive solar irradiance measurements.

Beneficial Aspects of Chaos in Fluid Mixing Presented

In recent years, dynamical chaos has been documented in many examples in physical, chemical, and biological systems. In most practical applications, chaos is detrimental and should be minimized or avoided altogether. In a seven-page featured article in the August 7, 1992, issue of Science, Professor J. M. Ottino of Northwestern University and his coinvestigators describe a variety of counterexamples where chaos is beneficial such as in the mixing of immiscible fluids. The article presents recent theoretical developments applicable to the interpretation and design of mixing processes in natural science and engineering. The Engineering Research program in DOE's Office of Basic Energy Sciences was a principal source of support for this research.

The mixing of fluids is a purely geometrical phenomena which is intimately bound to the stretching and folding of fluid elements, which, in turn, can lead to chaos. It has been shown experimentally and computationally that real fluid flows can produce the type of stretching and folding that leads to chaos, and provide a point of confluence and visual analog for chaotic behavior, multiplicative processes, and scaling behavior. The theory developed anticipates the coexistence of order and disorder - symmetry and chaos - and self similarity and multifractality arising from many stretchings and foldings. The concepts are useful in flow classification, design of mixing devices, enhancement of transport processes, and control of structure formation in two-phase flow systems.

Electroincineration Renders Organic Wastes Harmless

An Ames Laboratory chemist has demonstrated (July 1992) the first example of a fast and complete electroincineration of a toxic family of organic compounds. Electroincineration is a term used to describe the electrochemical oxidation of organic waste materials to harmless by-products (CO_2 and hydrogen ions). Supported by BES's Division of Materials Sciences to understand fundamental aspects of electrocatalytic oxidation of toxic chemicals, Dennis Johnson has discovered new, inexpensive, and rugged electrode materials and techniques for the fast and complete electroincineration of benzene and its derivatives. Benzene, a carcinogen, is a ubiquitous and troublesome chemical waste. The materials which Dr. Johnson uses are doped films of PbO_2 (lead dioxide); dopants can be various metal cations such as bismuth (Bi^{5+}), iron (Fe^{3+}), and silver (Ag^+). Currently, the electroincineration is a two-step process. Research will soon begin to test the possibility of converting benzene to CO_2 in a one-step process at a PbO_2 film doped with Fe^{3+} and Bi^{5+}.

Substantial interest has been shown for the use of these techniques to detoxify photographic wastes (Kodak), for carbohydrate waste removal in the starch processing industry, and for pesticide waste. Many other uses are likely, particularly because of the potential for fast, complete, and inexpensive detoxification of toxic chemicals.

"Out of This World" Chemical Compound Observed

The Wall Street Journal reported on July 13, 1992, that "the chemical compound, called positronium hydride, existed for a brief moment in a laboratory in Denmark." Positronium hydride is a hydrogen molecule with one of its two protons replaced by a positron. The Journal stated "Positronium hydride is the first of what may be a series of other worldly compounds that an American chemist, David Schrader of Marquette University, and his Danish colleagues hope to create in the laboratory by combining two contradictory atomic elements, particles and anti-particles." In actuality, the first discovery of the positronium hydride was reported 2 years earlier in Physical Review B, 41, 6220 (1990) by a team of Spanish scientists, R. Pareja, R. Gonzalez and their students, and an American physicist, Yok Chen of Oak

Ridge National Laboratory (ORNL). Dr. Chen is currently with the Department of Energy, Office of Basic Energy Sciences/Division of Materials Sciences (DOE/BES/DMS) on a half-time basis. Although the research itself was supported by the Comision Asesora de Investigacion Cientifica y Tecnica of Spain and Defense Advanced Research Projects Agency of the USA, the process by which the traps were introduced into the MgO crystal to capture the positrons to form positronium hydride was developed at ORNL under DOE/BES/DMS auspices and patented. The material in which positronium hydride was first observed was prepared at ORNL, and the first observation of the positronium hydride occurred in Madrid, Spain. The lifetimes in the two studies were the same: 5×10^{-10} second. The trapping hosts were different: hydrogen-laden MgO crystal in the initial discovery and methane in the recent study.

Quantitative Image Analysis Helps Determine Rock Properties

Fluid movement in rock and soil pore space is important in hydrocarbon production and monitoring and remediation of contaminated groundwater. Geophysicists at Lawrence Livermore National Laboratory (S. Blair and J. Berryman) have developed a rapid and economical method for obtaining permeability and other rock properties by characterizing the fine-scale geometric structure of pores. The method is based on statistical properties of the rock microgeometry as observed in Scanning Electron Microscope images of rock cross-sections. Spatial correlation functions derived from the images can be used to bound permeability, specific surface area, and other rock properties. Of particular importance is the extension to treat cases involving two fluid phases of contrasting wetting characteristics. The same basic approach, using spatial correlation functions, underlies a new research effort at Brookhaven National Laboratory (NSLS) involving x-ray computed microtomography to assess pore structure of geologic materials. (Proc. 32nd U.S. Rock Mech. Symp., 1991)

Effects of Forced and Natural Convection on the Unidirectional Solidification of Multicomponent Substances

At the Tenth Symposium on Energy Engineering Sciences, May 11-13, 1992, at Argonne National Laboratory, Professor F. P. Incropera of Purdue University presented experimental and numerical results on the effects of transport phenomena on the unidirectional solidification (UDS) of multicomponent substances. Convection is typically driven by buoyancy forces and, for multicomponent substances solidified under off-eutectic conditions, such forces originate from constituent composition gradients, as well as from thermal gradients. The convection is not restricted to regions of pure liquid (the melt) but may also occur in two-phase (mushy) regions consisting of a liquid-saturated, dendritic solid. A double-diffusive instability was bound to occur at the interface between fully liquid and mushy regions. One of the solidification schemes used involved chilling a multicomponent melt from below inducing upward propagation of the solidification front, (termed unidirectional solidification) which created columnar crystalline structures with a high degree of directional strength.

The UDS process may be used to develop high strength, light-weight super alloys for high temperature applications. The result may be of interest in materials processing as it relates to static casting of binary alloys, and in understanding and quantifying unacceptable mechanisms. Physical mechanisms associated with convection during solidification are also of interest in a wide range of other disciplines as oceanography, and geology.

Life of Chromatographic Supports Extended by Novel Chemical Bonding Scheme

A novel approach for solving the classic stability problem of silica chromatographic supports was developed by Chemical Sciences investigators at the University of Delaware. The bonded hydrocarbon partitioning phase on the silica support is chemically attacked by the alkaline aqueous solvents which are used as the sample carrier. This deterioration of the partitioning phase from the chromatographic support is a pervasive problem in biomolecular separations at extreme pH's. Protein separations require a Ph range that is extended beyond the typical working limits of 2-8. The novel enhancement consists of bonding a non-absorbent C_3 moiety along with a long C_{18} absorbing hydrocarbon phase to the silica support.

Spectroscopic studies of chemically modified chromatographic surfaces under various solvent conditions showed that the bonded phase structure played an important role in chemical stability and partitioning characteristics of these systems.

The chemically bonded C_3 retards hydrolytic (chemical) attack of the silica, while the long chain hydrocarbon allows typical chromatographic performance. The C_{18} surface made from this scheme was found to withstand washing with either acid or alkaline solutions that heretofore have rapidly destroyed conventional column surfaces. The bonding scheme has general applicability to virtually all types of functional groups which have specific separation capabilities. Applications of this technique are currently being pursued in analytical, preparative, and process scale biochromatography, as well as capillary zone electrophoresis. An application for a patent has been filed. This is an example of fundamental studies impacting a mature technology.

Chemical Radical-Radical Reaction Studied by New Technique

Chemical reactions between radicals are of considerable importance in combustion of small hydrocarbon species. The rates of many of these reactions have been measured directly and used in models of combustion systems. However, products of the reactions are frequently more difficult to determine. For example, the reaction of CH_3 + O has been extensively studied and the only reported products are H_2CO (formaldehyde) + H. The methods used previously to study this reaction were not sensitive to some products, such as CO or H_2, which can be a highly exothermic channel. In recent work, supported by the Chemical Sciences Division at the University of Colorado, methyl radicals and O atoms are prepared simultaneously and products observed with time-resolved Fourier Transform Infrared analysis (FTIR). In addition to observing formaldehyde, vibrationally excited CO is characterized as a direct product of the reaction. The definitive proof of the CO + H_2 + H channel has very important implications for combustion, since about 40% of the reaction bypasses formaldehyde and forms the more highly oxidized species CO, thus, eliminating several additional oxidation steps completely. The work also implies that the mechanism proceeds through CH_2OH (via reorganization) or HCO + 0_2, which then goes on to form CO. Additional theoretical work will be necessary to define the pathways in this system.

Novel Resonance Ionization Detector Developed

A novel resonance ionization detector which combines both ultra high resolution and extremely high sensitivity for photons has been developed by Chemical Sciences investigators from the University of Florida-Gainesville.

This design could prove advantageous over the typical monochromator/photomultiplier spectrometer system used today, which is limited by the trade off between resolution and sensitivity. The photon detector is based on the two-step laser-enhanced ionization of magnesium in a miniature acetylene/air flame. This research was presented at the RIS-92 (Resonance Ionization) Conference in Santa Fe, New Mexico, and was awarded the best poster at the conference, based on overall science and presentation. The work is based upon the 285.2 nanometer resonance absorption of magnesium in a two-step process, in which the flame serves as an atom reservoir for magnesium in its ground state. This resonance absorption captures incoming photons and a second laser is used to enhance the magnesium ionization for detection. The minimum detectable number of photons in the present design was determined to be 1000. It is hoped that in the future this number can be lowered even further. The poster demonstrated the use of the resonance ionization detector to detect the scattered photons from the Raman spectrum of dimethylsulfoxide. Possible applications for this type of detector could be in long distance fiber optic communications in high light environments.

Novel Gas Phase Ion Chemistry Discovered

Chemical Sciences investigator, Dr. Ben S. Freiser at Purdue University, has discovered a naked bimetallic cluster ion, $MgFe^+$, which demonstrates unique reactivity. This heteronuclear diatomic ion reacts with linear alkenes by magnesium displacement to form a Fe^+-olefin product and with alcohols by iron displacement to form a Mg^+-alcohol product. This is the first reported example of a changeover in the relative metal-ligand bond energies with both metals in a dimer being selectively displaced. Professor Freiser is using Fourier transform mass spectrometry coupled with laser ablation to study the gas phase ion chemistry of these bimetallic ion clusters. This technique is ideally suited for the study of gaseous ion chemistry because of its capability for storing ions for long periods of time, up to tens of seconds. Fundamental information can be obtained on such basic parameters as ion structure and thermochemistry, as well as on the effect of photon absorption on ion reactions. These metal cluster systems provide information which can be applied to a wide range of disciplines, including catalysis, surface science, atmospheric chemistry, and analytical mass spectrometry.

Argonne National Laboratory Team Publishes Research on Molecular Electronic Switches

The July 3, 1992, issue of Science reports a significant advance toward miniaturizing electronic circuits to the molecular scale by a research team in the Chemistry Division of Argonne National Laboratory. The team has designed a molecule that acts as a picosecond electron switch when exposed to short pulses of visible light. The switch is very fast because it involves electron transfer and no molecular motions. The molecule consists of two porphyrin rings joined by a long dicarboximide bridging group. This donor-acceptor-donor molecule exhibits light intensity-dependent optical switching by means of two ultrafast electron-transfer reactions: as the light intensity is increased, the molecule switches from being a strong transient absorber at a wavelength of 713 nm to an absorber at 546 nm. The dicarboximide bridging group is a photostable electron acceptor that has been used in dyes, electrophotography, and liquid crystals. The authors conclude that this achievement opens up the possibility of developing molecular electronic devices based solely on electron motion within donor-acceptor complexes. The work is being supported by the Division of Advanced Energy Projects/Basic Energy Sciences and the Exploratory Research Fund of Argonne National Laboratory; Michael R. Wasielewski, principal investigator. (Science 257, 63, 1992).

Symposium on Ceramic Synthesis and Processing Published

The proceedings of the Materials Research Society Symposium "Synthesis and Processing of Ceramics: Scientific Issues" have been published by the Materials Research Society. The Symposium took place on December 2-6, 1991, in Boston, Massachusetts, was co-sponsored by the American Ceramic Society and financially supported by the Office of Naval Research, Martin Marietta Energy Systems and Corning. The published proceedings consist of 79 peer reviewed manuscripts. The symposium organizers and proceedings editors were W. E. Rhine of Massachusetts Institute of Technology, T. M. Shaw of IBM, Yok Chen on assignment to Materials Sciences from Oak Ridge National Laboratory and Bob Gottschall from Materials Sciences.

Publication Accepted on Workshop on Computational Issues in the Mechanical Behavior of Metals and Intermetallics

Improved computational methods for predicting the mechanical behavior of metallic alloys and intermetallics is of critical importance to the National Energy Strategy for four broad reasons. First, the efficiency of energy conversion and conservation systems is limited by the extremes of system environmental parameters (temperature, applied stress, derivative of applied stress with respect to time, and reactive environment such as hydrogen, etc.). It is, therefore, necessary to develop new alloys and intermetallics that can safely withstand yet higher extremes of such hostile environmental parameters in order to achieve performance improvements in energy conversion and conservation systems. Second, it is necessary that load bearing components perform without dimensional change or fracture in such hostile environments for reasons of human safety. Fracture resistance is also necessary for the safe containment of hazardous species in energy conversion and conservation systems and hazardous or toxic species transport and containment. Third, an improved predictive capability is necessary to achieve early warning of impending catastrophic changes in dimensions or fracture, so as to permit early retirement of critical safety-related components at the time of routinely scheduled shut-down periods. Fourth, the capability to mechanically deform or "work" alloys and intermetallics into useful shapes and forms that are without property-degrading flaws and defects is an absolute necessity.

In response to the above concerns, a workshop entitled "Computational Issues in the Mechanical Behavior of Metals and Intermetallics" was held on September 30 - October 3, 1991. The starting point for this workshop was the recognition that new atomistic and continuum methods, coupled with the emergence of more powerful computational facilities, now make possible the design of new alloys and intermetallics and the prediction of the properties and behavior of existing ones. The syllabus for this workshop and the report on its findings fell quite naturally into four topical areas which span the spatial scale relevant to mechanical properties and behavior: (1) atomistics, (2) dislocations/interfaces, (3) microstructure, and (4) the (elastic or plastic) continuum. It included a crosscut exercise that crossed the expertise of scientists that are leaders in computational methods for each of these regimes of the spatial scale with those with expertise in four generic topics that are critical to the DOE mission: (1) instability phenomena, (2) composite interfaces, (3) high temperature phenomena, and (4) intermetallics.

A general, but key, recommendation from this workshop was for recognition in both the technical community and in government program offices that computational materials science requires synergistic contributions from researchers working on phenomena occurring at all spatial scales from atomistic to continuum. Other needs that were identified included realistic potentials for diverse alloys and intermetallics including impurity interactions, a library of potentials, general methods to expand the molecular dynamics time regime by ten orders of magnitude (required for time-dependent engineering behavior), general coupling methods between discrete (with dislocation singularities) and continuum computations, and experimental verification of computations at all spatial levels.

This workshop was supported by the Division of Materials Sciences and organized by Dr. M. I. Baskes of Sandia National Laboratories. The summary report was written by Baskes, Professor R. G. Hoagland (Washington State University) and Professor A. Needleman (Brown University). The report has been accepted for publication as the keynote article in Materials Science and Engineering. The 24 scientists that participated in the workshop were drawn from a wide spectrum of expertise from universities, DOE and other national laboratories, and industry.

Mechanisms of Damage Growth in Semiconductors is Better Understood

The growth of damage produced during ion irradiation of semiconductors such as GaAs, Si, Ge and Si-Ge alloys has been shown to occur as a result of two distinctly different growth mechanisms which dominate in different temperature regimes. The transition between these regimes occurs at a temperature which depends upon the particular substrate material and, to a lesser extent, the ionic species. The transition is marked by a dramatic decrease of the damage yield per incident ion as temperature is increased over a narrow range near the transition temperature. The model which describes the behavior is based upon a low temperature mechanism of prompt reaction to the displacement events along the ion track; damage formed in this way is localized to a volume surrounding the ion track and the yield is independent of the ion flux. At higher temperatures, the damage is attributed to a mechanism of delayed interactions between mobile, primary defects which survive cascade quenching. Thus, the transition temperatures, which vary between 40 °C (GaAs) and 150 °C (Ge), are determined by the mobilities of the defects in different substrates. Because ion implantation is an important tool for providing controlled doping of semiconductors for electronic and optical device applications, the results are important to the development of effective semiconductor processing procedures.

The research was completed in early 1992 by T. Haynes and W. Holland in the Solid State Division of Oak Ridge National Laboratory.

Three-Dimensional Imaging Obtained of Fault-Zone Velocity Structure

Seismologists at the Lawrence Berkeley Laboratory (LBL) Center for Computational Seismology reported in June 1992 that numerical codes they have developed and implemented are being widely used to support DOE applications in Geothermal, Defense, and Environmental Restoration Programs, as well as research applications in other national programs. The computational codes are used to obtain three-dimensional subsurface images of heterogeneous geological features (such as faults, geothermal reservoirs, subsiding oil fields and active volcanoes) from seismic waves generated by earthquakes or by explosives. One recent illustration was the method developed and tested using data from microearthquakes along the highly instrumented Parkfield segment of the San Andreas Fault in central California, and the results provide a three-dimensional velocity model for this portion of the fault. A 2-km-wide volume near the location of the 1966 earthquake hypocenter presently has seismic characteristics indicative of high fluid pressures. This zone, which is considered a possible nucleation site for a future earthquake, is under intense study by the LBL group as well as by many other researchers. The Geosciences Program in Basic Energy Sciences provides core support, supplemented by individual project funding from DOE and other sources, for the LBL Center for Computational Seismology. Data acquisition for the Parkfield project is supported by the U.S. Geological Survey.

Boron Nitride Synthesis Accomplished at Low Temperature

In an unusual application of synchrotron radiation, scientists at the Brookhaven National Laboratory (BNL) used light from the National Synchrotron Light Source to form hexagonal boron nitride (BN) films from a mixture of diborane (B_2H_6) and ammonia condensed on a silver substrate at 78K. The cryogenic technique provides a great increase in reactant density in the reaction region. While diborane and ammonia interact at 78K, the formation of the BN layer only occurred upon exposure to the "white" synchrotron light. This mechanism provides a natural way to pattern a BN film using synchrotron radiation-based or vacuum ultra-violet and soft X-ray lithographic processes. With source wavelengths on the order of 1 nm, relatively small BN structures are possible. The research was supported by the Division of Materials Sciences and performed by D. R. Strongin, J. K. Mowlem, M. W. Ruckman, and M. Strongin of BNL. The results were obtained in late 1991.

Giant X-ray Absorption Circular Dichroism Observed

Extraordinarily large circular dichroism has been observed in the near-edge X-ray absorption of monolayer films of iron on a face of single crystal copper by researchers at Lawrence Livermore National Laboratory (LLNL) working cooperatively with a scientist at the IBM Almaden Research Center. The effect was observed while investigating the differential absorption of circularly polarized synchrotron radiation as a function of magnetization in the film. The effect, labeled perpendicular dichroism because both the magnetization and X-ray incidence are normal to the surface, is a direct measurement of the spin polarization and the density of unoccupied states near the Fermi energy in a ferromagnetic system. The experimental parameters also permit an approximate determination of the magnetic moment. This is the first reported observation of perpendicular dichroism in a metal overlayer. The experiments were performed at the Stanford Synchrotron Radiation Laboratory.

The research was performed by J. G. Tobin and G. D. Waddit at LLNL and D. P. Pappas of IBM; the results were published in Physical Review Letters in June 1992.

Fluidity Limits of Energy-Related Suspensions Correlated With Random Packing of Dry Solids

As reported in the March 2, 1992, issue of Physical Review Letters, Professor Ronald F. Probstein of MIT investigated the fluidity limit by studying the viscosity of concentrated non-colloidal monodisperse and bidisperse suspensions of hard spheres. The fluidity limit is that volume fraction of the solid phase below which the suspension behaves like a liquid. He also inferred the maximum packing fraction by extrapolation from rheological experiments in which the viscosity of the suspension is measured as a function of solid fraction.

The lower bound of the high shear rate fluidity limit was measured for monodisperse and bidisperse suspensions of spherical particles. The existence of a correlation between the fluidity limit and random packing of the dry solid fraction was demonstrated. The ratio of the random-close-packing fraction to the lower bound fluidity limit of the bidisperse suspension was found to be the same as for monodisperse spheres, a constant of 1.19 suggesting a random structure at this limit. This correlation allows the rheology of concentrated suspensions to be determined by simple dry packing measurements independent of viscosity experiments.

The results obtained are expected to provide a rational predictive methodology for describing the rheological and flow properties of polydisperse, dense-phase slurries which will assist in the development of new technologies for efficient transportation, handling, and utilization of suspensions, such as coal-water, cool-oil, drilling fluid-muds, and scrubber sludge slurries. Designs involving slurry transport in the energy industry will be enhanced.

Findings of Materials Sciences-Sponsored Workshop on Intermetallics Submitted for Publication

The high strength and low ductility (and hence fabricability) of ordered intermetallic compounds have been well known for over 60 years. The strong tendency for chemical ordering in ordered intermetallics is derived from the fact that the bonding between dissimilar constituent atoms is greater than that between identical atomic species. The physical consequences of this strong chemical bonding include good stability of superlattice crystal structures; reduced atomic mobility and, therefore, reduced creep rate at elevated temperatures; and reduced dislocation mobility. The reduced mobility of lattice dislocations leads to increased resistance to plastic deformation, poor ductility and inherent brittleness in polycrystalline ordered intermetallics at room temperature, and thus poor fabricability into useful engineering shapes.

The Division of Materials Sciences sponsored a workshop on the "Deformation and Fracture of Intermetallics" in September 1991. This workshop identified research needs and opportunities that would lead to answers to critical issues concerning intrinsic strengthening mechanisms at elevated temperatures and inherent brittleness. Four principal findings were: 1. Brittle-to-ductile transition (BDT) behavior (i.e., cleavage strength, grain boundary strength, crack-tip plasticity and transformation) should be investigated experimentally and interpreted theoretically, including the effect of strain rate on BDT temperature in terms of atomic diffusion and dislocation mobility. 2. Measurements of critical parameters (e.g., diffusion coefficients, shear fault energies, etc.) and studies of grain boundary structure and chemistry are needed for better understanding of the unique physical and mechanical properties of ordered intermetallics. These studies would benefit from the strengthening of DOE facilities for crystal growth and microstructural characterization. 3. Improved theoretical techniques should be developed to bridge the gaps among electronic structure, atomistic simulations, dislocation micromechanics, continuum mechanics and microstructural modeling. 4. Novel material synthesis and processing techniques should be developed to control microstructures to obtain optimum mechanical properties of monolithic and/or multiphase intermetallic systems. Such techniques together with characterization studies form the basis for developing comprehensive understanding of structure-properties relationships. The organizers of this workshop were Dr. M. H. Yoo (Oak Ridge National Laboratory), Dr. S. L. Sass (Cornell University), and Dr. J. B. Darby, Jr., of the Materials Sciences staff. As with most BES workshops, the invited participants invoked expertise from universities, DOE laboratories, and private sector industry. There also was scientific representation from an Air Force Laboratory and from abroad. The report of this workshop was submitted in June 1992 for publication in a refereed journal.

Dissolution Rates of Minerals Controlled by Metal-Oxygen Bonds

Silicate minerals, the most common rock and soil-forming minerals in the Earth's crust, react with aqueous fluids and dissolve at widely different rates. In Nature (January 9, 1992) Bill Casey (UC-Davis) and Henry Westrich (SNL), supported by the Geosciences Program, presented data on factors controlling rates of dissolution of orthosilicate minerals. These minerals, such as olivine, are characterized by isolated SiO_4^{-4} tetrahedra and represent an important limiting class of minerals. Dissolution rates for alkaline-earth (Ca, Mg, Be) orthosilicates increase with cation radius. Those containing transition metals, of very similar ionic radius, show dissolution rates decreasing linearly with increasing number of cation *d* electrons. Both types of behavior are consistent with control of dissolution rate by the nature of the cation-oxygen bonds. Understanding of such phenomena is important in predicting the rate and nature of mineral-fluid interactions related to energy resource use and mineralogical sequestering of environmental contaminants.

Theory Predicts Unexpected Molecular Effects at High Laser Intensity

The making and breaking of chemical bonds are critical to understanding chemical processes and the concept of a bond strength underpins this understanding. The strength of the bond, if fact, has its foundation in standard thermodynamic quantities. However, new developments in the study of nonlinear effects using high intensity lasers in atomic physics may require a fresh look at the concept of a unique chemical bond energy, a review not unlike that prompted by the discovery of "above threshold ionization." Now, new theory developed by Professor Shih Chu of the University of Kansas, with support of the Chemical Sciences Division, predicts that chemical bonds, as in H_2^+, may be "softened" in the presence of intense photon fields leading to efficient photodissociation of low-lying vibrational levels. The same theory predicts the "hardening" of molecular bonds involving high-lying energy states resulting in laser induced stabilization of molecules in intense laser fields. These counter-intuitive results appear at very high, but experimentally attainable, laser field intensities where the potential energy field of the molecule and the laser field interact cooperatively to yield new phenomena which neither field can produce by itself. This discovery is expected to have broad applicability to improving our understanding of behavior in other scientific areas.

Synthetic Diamond Coatings Grown Using "Buckyballs"

The research of Professor R. P. H. Chang of the Department of Materials Science, Northwestern University, was cited in articles in the November 6, 1991, issue of The Wall Street Journal and in a November issue of Science. Professor Chang's investigation of the growth of diamond films by chemical vapor deposition (CVD) is partially funded by the Department of Energy's Division of Materials Sciences. Under the Department of Energy support, Professor Chang has investigated substrate effects on film growth and the fundamental problem of film nucleation which are among the most significant technical and scientific problems in diamond film growth. Professor Chang and his colleagues recently found that film growth could be nucleated with the C_{70} molecular form of buckyballs. A silicon substrate was coated with a C_{70} film which was then ion bombarded to open from a diamond film consisting of many ultrafine diamond crystallites. Professor Change reported that the quality of the C_{70} nucleated diamond film is comparable to the best films produced to date by other methods. He also reported that diamond films cannot be grown successfully if the C_{60} molecular form of buckyballs is used as nucleation sites.

Diamond films are typically grown on surfaces which have been abraded or which have been dusted with a fine diamond grit. CVD growth on such surfaces yields a diamond film consisting of many ultrafine diamond crystallites. Since it is difficult to control the uniformity of the abrasion or the diamond grit coating, the resulting diamond film growth may not be uniform in either coverage or texture. Growth on a C_{70} prepared surface offers the possibilities of obtaining a more uniform film and of growing diamond films on curved surfaces. Furthermore, the successful growth of polycrystalline diamond films on ion-bombarded C_{70} treated substrated may bring the research community one step closer to the growth of continuous single crystal diamond films. Professor Chang and his colleagues have developed a simple model for explaining their observations. The detailed mechanism for the C_{70} assisted growth is currently being studied.

Fundamental Robotics Research Helps Human Genome Program

A basic problem facing autonomous robotic systems is the reconciliation and integration of data from multiple sensors, so-called sensor fusion, needed for decision making. That is accomplished by techniques such as neural networks and fuzzy logic.

Recently, research on those techniques, supported by the Engineering Research Program at the Center for Engineering Systems of Advanced Technology (CESAR) project, came to the attention of Dr. E. Uberbacher, a biophysicist at the Oak Ridge National Laboratory (ORNL). Inspired by the ideas at the base of those methods, he and members of his group, including some CESAR-ORNL staff, partially supported by the DOE Office of Health and Environmental Research, have created a novel and highly effective software for human DNA sequencing. The software package, Gene Recognition and Assembly Internet Link (GRAIL), can find 90% of the genes very quickly using a PC, rather than a supercomputer. As an example, preliminary results point to the location of the gene responsible for Huntington's disease, although the gene itself is still elusive.

GRAIL is now in use by over 300 genome research laboratories worldwide. ORNL is in the process of negotiating a CRADA with Intelligenetics, Inc., aimed at better exploiting this software.

Fundamental Aqueous Chemistry Studies of Corrosive Steam Benefits Geothermal Energy Program

Modeling of the complex chemical behavior of natural systems is often limited by the availability of fundamental thermodynamic information concerning the components of the system. An example of such a problem is the assessment of possible sources of corrosive hydrogen chloride (HCl) gas in the natural steam at The Geysers geothermal energy field in California. This field is being developed with assistance from the Office of Renewable Energy Conversion, CE-12, and the problem of steam corrosion is directly impacting the success of the program. New measurements by the Chemical Sciences-supported aqueous chemistry group at the Oak Ridge National Laboratory of the volatility of HCl from aqueous solutions at elevated temperatures now permit the modeling of plausible sources of HCl found in the steam. The new data were combined with earlier measurements of HCl and brine solutions to obtain the needed expression for the liquid-vapor partitioning of HCl. Values for HCl partitioning calculated from the new model differ from earlier values, based on measurements from much lower temperatures, by more than a factor of 100. This work will allow quantitative predictions to be made of the corrosive and fouling behavior of HCl and other solutes in steam from both natural sources as well as power plants, and the DOE geothermal energy development program is an immediate beneficiary of this new capability.

New Synthesis of Corannulene Achieved, Providing a Structural Subunit of "Buckminsterfullerene"

"Corannulene," the bowl-shaped primary subunit of the new C_{60} form of carbon known as "Buckminsterfullerene" has become available by a remarkably short and convenient laboratory synthesis devised by Chemical Sciences supported researchers at the University of Nevada, Reno. This widely sought goal also marks the first time a convex polycyclic aromatic hydrocarbon (PAH) has been prepared by the molecular strategy of converting a natural planar fluxional molecule to the less stable nonplanar form. The ^{13}C NMR spectrum of corannulene was also reported for the first time. The only prior synthesis of corannulene was reported 25 years ago by a lengthy, torturous, and low-yield route, but further exploration of its potentially fascinating chemistry could not be explored due to its lack of availability. Now, by a clever combination of conventional chemical transformation and a novel gas phase thermal rearrangement reaction, the first well-defined example of the capture of a planar PAH in a temporary nonplanar geometry to build a convex surface was demonstrated. The thermal flash vacuum pyrolysis entailed a sudden heating to 1000 °C which trapped the less stable form of the PAH.

Recent interest in corannulene centers about its structural relationship to the new spheroidal form of elemental carbon (buckyball, C_{60}), since corannulene can be viewed as the carbon framework that comprises the "polar caps" of C_{60}. Now that corannulene is readily available, the possibility exists to join two or more molecules together to make Fullerene-type molecules in a controlled fashion, possibly with metals or other guest molecules trapped within. Further extensions of the new high temperature cyclization principles include the preparation of other curved surfaces and larger structural subunits of C_{60}, such as baskets and tubes.

The recent report on the new synthesis of $C_{20}H_{10}$ has enabled the molecular dynamics of this interesting polycyclic aromatic hydrocarbon to be measured. The results were featured in a cover article of Chemical and Engineering News. Variable temperature nuclear magnetic resonance (NMR) spectroscopy has indicated that the barrier to inversion of the corannulene ring system, i.e., the energy required to flip the corannulene bowl inside out, was very low, about 10 kcal/mol at -90 °C. This would be equivalent to the bowl-shaped molecule inverting more than 200,000 times per second at room temperature!

The very rapid interconversion has surprised most chemists who thought the corannulene molecule would be quite rigid since it had to pass through the very stable planar configuration. Indeed, some calculations on the energy differences between bowl and planar conformations had ranged to over 70 kcal/mol, indicating a very rigid structure with an interconversion half-life of many centuries. Professor Scott of the University of Nevada, Las Vegas, is continuing to explore the fascinating chemistry of even larger polycyclic bowls and their complexing ability with metals, and believes that his procedures may be useful for synthesizing a variety of fullerenes.

Novel Swirl Burner Development Opens Opportunities for Potential Technology Transfers

Chemical Sciences combustion researchers at the Lawrence Berkeley Laboratory have developed a novel swirl burner for premixed flames that has the potential for significant technology transfer. A simple swirl generator attachment to a regular flame burner was found to stabilize lean flames which, at low temperatures, reduce the formation of polluting nitrogen oxides. The most significant aspect of the discovery is that, under conditions of weak swirl, freely propagating yet stationary flames can be stabilized. The stabilization occurs because of divergence of the flow which expands by centrifugal force, causing the flow velocity to decrease naturally. The flame maintains itself at the position where flow velocity equals the flame speed. This is a very stable flame propagation condition and flame blow-off is effectively prevented. Also, the burner operates under a much broader range of mixture conditions than other existing burners.

A patent has been applied for this modified burner concept. Developing the burner for home furnace use seems like the logical first application, either as a replacement burner or as a retrofit. In addition to commercial applications, the burner is attractive for research because the swirl stabilized flame is adiabatic and much more accessible to probing by laser methods. This makes it ideally suited for investigating the details of the fundamental processes of combustion chemistry, materials synthesis, and waste incineration. This also opens up studies of lean combustion which were not previously possible because of flame instabilities. Future work by the LBL group will include: (1) the study of chlorofluorocarbon incineration by means of the new laminar burner; and (2) extension of the swirl burner studies to higher turbulence levels to determine the effects on flame stability and quenching.

A New Class of Silicon Nitride Ceramics Show Improved High-Temperature Properties

A new class of silicon nitride ceramics with improved resistance to oxidation and better strength at high temperatures has been developed by tailoring microstructures to the demands of the anticipated service environments. These new materials are produced through the use of rare-earth oxides in place of the alumina-yttria mixtures added to traditional silicon nitride powders to promote densification during sintering. Through suitable heat treatments, the glassy grain boundary phases formed by these new additives can be transformed through devitrification to highly refractory rare-earth disilicates. This conversion to crystalline grain boundary phases significantly decreases the loss in high-temperature strength associated with softening of amorphous grain boundary phases. Lanthanide-oxide sintered materials which show improved performance can retain up to 91% of room temperature flexural strength at 1300 °C. In addition, the newly designed microstructures improve creep resistance at high temperatures. The gradual decrease in creep rates with time is attributed to continued devitrification of residual glassy phases destabilized by outward diffusion of impurities. Oxidation resistance is also improved by a factor of 10 compared to what is observed in traditional silicon nitrides. This improvement is attributed to reductions in the diffusion rates of additive and impurity cations in the crystalline grain boundary phases.

The improvements in high temperature behavior realized with this new class of silicon nitrides represent an important step towards the application of ceramics in next-generation turbine and reciprocating engines. These engines will be required to operate at extremely high temperatures to meet expected efficiency and cleanliness standards. This work, under Professor Gareth Thomas and Dr. M. K. Cinibulk, is continuing at the Center for Advanced Materials at Lawrence Berkeley Laboratory to evaluate other mechanical properties of these lanthanide-oxide sintered materials, such as their resistance to the initiation and propagation of cracks in the presence of the small flaws inherent in ceramics.

Discovery of New Electrolyte Permits Development of Improved Rechargeable Lithium Battery

Research on noncrystalline lithium-ion-conducting solid electrolytes has been largely confined to oxide, sulfide, and mixed oxide-sulfide systems. Although several glasses in these systems have high conductivities, none are stable in contact with lithium and so cannot be used in primary or secondary lithium batteries. A new amorphous lithium electrolyte that is stable in contact with lithium and has a good ionic conductivity has been synthesized in thin-film form by rf magnetron sputtering of lithium orthophosphate, Li_3PO_4, in pure nitrogen. The composition of the new material has been determined to be approximately $Li_{3.3}PO_{3.9}N_{0.17}$, and its lithium ion conductivity at 25 °C is 2×10^{-6} S/cm. When Li_3PO_4 is sputtered in $Ar + O_2$ process gas mixtures, the resulting films, which have the composition of $Li_{2.7}PO_{3.9}$, are not stable in contact with lithium and have conductivities at 25 °C that are nearly two order of magnitude lower. The stability toward lithium and the higher ionic conductivity achieved by incorporating less than 5 atomic per cent nitrogen into the amorphous lithium phosphate films is not completely understood at this time. However, optical and photoelectron spectroscopic studies suggest that it is due to a crosslinked network structure formed by the bonding of three phosphate groups to a nitrogen.

The discovery of the oxynitride lithium electrolyte has made possible, for the first time, the development of a solid state thin-film rechargeable lithium battery that does not require an extra film of LiI to protect the electrolyte from attack by lithium. The battery consists of a lithium anode, the oxynitride electrolyte, and an amorphous vanadium oxide cathode, VO_x, with x approximately 2.5. Depending on the exact value of x, the open circuit voltage of the cell is between 3.6 and 3.8V, the highest of any on record. The battery has potentially many applications as an active or standby power source for low-current electronic devices such as CMOS static random access memories. This research was performed by J. R. Bates, N. J. Dudney, G. R. Gruzalski, and R. A. Zuhr of the Solid State Division; A. Choudhury of the Metals and Ceramics Division, Oak Ridge National Laboratory; and J. D. Robertson of the University of Kentucky. A joint project with Eveready Battery Company under a CRADA is being formed to develop a packaging technology for thin-film lithium batteries.

High-Density Alloy Produced by Reaction Sintering Processes

The aluminide, Ni_3Al, was produced by reaction sintering using elemental powders (i.e., nickel and aluminum powders). Existing reaction sintering processes produce Ni_3Al alloys generally containing 2 to 5% porosities, which substantially reduce the mechanical properties of the alloys. In a study by C. Nishimura and C. T. Liu at Oak Ridge National Laboratory, the reaction sintering was carefully controlled by applied stresses, and microstructures and phases were characterized by electron microprobe. It was discovered that both reaction kinetics and products are extremely sensitive to compressive stresses applied to green compacts during sintering processes at 620 °C. A control of loading modes and stresses leads to successful products of high-density (99.3%) Ni_3Al material - the highest density ever reported for reaction-sintered Ni_3Al. It is important to point out that residual porosities observed in this case are extremely fine and also uniformly distributed in Ni_3Al. The beneficial effect of loading is believed to enhance heat flow which affects both reaction kinetics and solidification processes during reaction sintering.

Intermetallic compounds such as Ni_3Al are potentially new structural materials for high-temperature use. They are, however, difficult to fabricate into structural components by conventional techniques which require extensive plastic deformation. Therefore, the utilization of powder metallurgical processes, which preclude the fabrication problem, is of significant attraction and importance. Reaction sintering is a unique and attractive process to produce intermetallics using self-sustaining exothermic-reaction. The process has various advantages, including near-net shaping, energy saving, low cost, and short processing time. A major problem associated with this process is the generation of significant amounts of large pores, which substantially reduce the mechanical properties of intermetallics. The recent results reveal the possibility of obtaining high-density and near-net shaped Ni_3Al components by controlled reaction sintering processes. As a result, HIPing (a costly process) is not needed to reduce porosity in the material.

Novel Biological Sensors Developed to Diagnose Specific Molecules and Organisms

Lawrence Berkeley Laboratory (LBL) scientists are creating sensors able to lock onto and detect targeted molecules and organisms. Biologically sensitive thin films are being developed that serve as selective sensors in medical diagnoses. The best medical sensors currently available rely on cumbersome, time-consuming assay techniques to detect specific pathogens. When dealing with low concentrations of pathogens, they often are inaccurate. Conversely, the new sensors will detect low concentrations and provide immediate results. They will allow a doctor to make an on-the-spot diagnosis and a patient to receive the added benefit of more immediate medical care. The diagnostic devices rely upon bioelectronic thin films developed by a team led by Mark Bednarski and Jon Nagy of LBL's Center for Advanced Materials. The new films are possible due to recent advances in materials science. Researchers create the films with a micro-fabrication process called molecular self-assembly. The degree of molecular organization can extend beyond that achieved by etching with the photolithographic technologies used to create silicon semiconductors. The films are generated by manipulating the interactions between molecules, exploiting phenomena that range from van der Waals' interactions to entropy. Bednarski, Nagy, and Berkeley graduate student Troy Wilson have pushed molecular self-assembly well beyond its previous limits, becoming the first to fabricate complex molecules at the surface of films. In an important advance, the team has fabricated an array of molecules that bind to different pathogens as well as to an assortment of biological receptors, including complex carbohydrates and peptides. The scientists have described their work in a series of recent journal articles including an upcoming paper in the Journal of the American Chemical Society.

New Ultra-Sensitive Technique Developed for Detection of Molecules in Dilute Solutions

Chemical Sciences investigators at Oak Ridge National Laboratory have reported the capability to detect single molecules in solution. This technique involves the use of laser fluorescence detection combined with microdroplet levitation to count the number of fluorescent analyte molecules in very dilute solutions. The ability to determine whether an analyte molecule is present or not in the droplet is related to the fluorescent signal being "on" or "off" as in a digital switch. This technique presents a radically new way to quantitate very low concentrations and changes how one approaches the analytical determination of a molecule being present in a sample. The detection threshold can be set to find all analyte molecules. For example, when analyzing a highly toxic substance, missed molecules would be very undesirable errors while false positives would be less serious. This detection scheme was investigated using a strongly fluorescing biological molecule at an average concentration of 1.75 picoliters (10^{-12} liters) in levitated microdroplets of 9.5 microns diameter (approximately 0.45 picoliters volume).

Frequency of Large Magnitude Earthquakes Less Than Previously Estimated

A 1989 theoretical prediction by Lawremce Livermore National Laboratory geophysicist J.B. Rundle (while at Sandia National Laboratories) concerning the frequency of occurrence of large and great earthquakes (above magnitude about 8) has been independently confirmed recently by seismologists at Columbia University. A long-held notion, based on extrapolation of earthquake magnitude-frequency relationships, was that the rate of occurrence of all earthquakes from the smallest to the very largest followed a simple relationship, so that large earthquakes were thought to occur at a rate that is easily extrapolated from the rate at which small earthquakes occur. Rundle calculated, and the Columbia geoscientists confirmed, that very large earthquakes occur less frequently than the extrapolation from small earthquakes would indicate. Seismic hazard estimates for the destructive potential of great earthquakes need to be revised downward in view of the understanding of the lower frequency of occurrence of these large, damaging events.

Surprise Predictions Made of Systems With Unusually High Hydrogen-Storage Capability

Surprise predictions that a positively charged metal ion (for example, a Ni^+ ion) can bind as many as ten hydrogen molecules has been made by Materials Sciences grantees P. Jena and B. K. Rao of the Virginia Commonwealth University. Their findings, which are based on theoretical modelling of metal clusters, are described in a recent Physical Review Letters. The binding is governed by a charge polarization process. On the other hand, a negatively charged ion can trap hydrogen both in the dissociated state as well as in the molecular form. However, the number of bound hydrogen atoms is far less than that in the case of the metal cation. The neutral metal atom binds the least number of hydrogen. It was also pointed out that small metal clusters with high ionization potentials are more reactive with hydrogen than the ones with a low ionization threshold. The reverse is true for large metal clusters.

Experimental verification of this prediction will be important in the search for environmentally safe storage of energy. The ability of the positively charged ion to trap a large number of hydrogen atoms has important implications in problems associated with hydrogen storage, since ions can be isolated in matrices such as zeolites, and also can be expected to have implications in the understanding of heterogeneous catalysis.

A New Ion Exchange Resin Developed for Improved Treatment of Waste Streams

Chemical investigators have synthesized and characterized a new ion exchange resin that shows considerable potential for the removal of contaminant metal ions from groundwater and mixed waste streams. Interest in the development of improved methods for such water treatment continues to increase as current methods are hard-pressed to meet the more stringent environmental laws and lower permissible discharge limits. This new resin has been dubbed "Diphonix," which stands for diphosphonic ion exchange, indicating that the strongly complexing moiety is an alkyl-1,1-diphosphonic acid group attached to an organic polymeric matrix. This material shows a strong affinity for actinides because of the strong bonding between the metal ion and the diphosphonic acid group, even in very acid media. In addition, this resin has had favorable results with other heavy, toxic metal ions such as zinc, cadmium, mercury, and lead in hard water and highly salted solutions. A single resin with such a broad range of capabilities has not been available heretofore. A patent application has been filed by ARCH Development Corporation and licensed to EIChroM Industries, Darien, IL, which has started commercial production. Preliminary tests by a major water treatment company are very favorable. This work was performed by the Argonne National Laboratory Chemical Separations Group led by Dr. Phil Horwitz in collaboration with Prof. Spiro Alexandratos of the Chemistry Department, University of Tennessee. The basic research on the principles of chemical separations is supported by the Division of Chemical Sciences. The collaborative resin development and characterization effort is supported by the Division of Advanced Energy Projects.

A New Method is Developed for Dating Groundwater History

An Argonne National Laboratory geoscientist (N.C. Sturchio) has established the feasibility of dating travertine formations up to 8,000 years old, using naturally occurring radium isotopes that are incorporated in the deposits when they form. Travertines are calcium carbonate deposits that precipitate from hot or cold spring waters in areas underlain by limestone bedrock. The Argonne study focused on travertines at Mammoth Hot Springs in Yellowstone National Park. Results of the study indicated that ^{222}Ra (half-life = 1600 years) can be used to calculate ages and deposition rates of deposits up to ~8000 years old. The shorter-lived ^{228}Ra isotope (half-life = 5.75 years) can be used to date travertines up to ~30 years old. The ability to date young travertines is useful in characterizing groundwater discharge history in relation to climatic and/or volcanic influences and allows predictions of future groundwater flow.

Neutron Diffraction Studies Improve Understanding of Residual Stress in Advanced Materials

Neutron diffraction offers a unique nondestructive method for examining the stress state of polycrystalline composites. The penetrability of neutrons in materials is usually measured in millimeters compared to microns for X-rays, so neutrons measure bulk rather than surface stresses. Neutron diffraction experiments at LANSCE were used to examine residual stresses produced during fabrication and deformation in aluminum and titanium silicon carbide composites. The results have confirmed the ability of numerical models proposed by scientists at Los Alamos National Laboratory and Brown University to make semiquantitative predictions of the internal stress state. However, intriguing differences exist between the experimental results and the model predictions. The experiments show the limitations of the computer simulations of residual stress. In addition, the neutron results have shown that X-ray measurements can be misleading because steep gradients can exist below the surface of continuous-fiber composites. The addition of ceramic reinforcement to lightweight metals results in materials with greater stiffness and tensile strength than the original metal. These metal-matrix composites are replacing conventional materials in structural applications that require high-strength or stiffness-to-weight ratios. Reduced weight gives improved efficiency and composites are already extensively used by the aerospace industry. As composites are considered for an increasing number of critical structural applications, the thermomechanical conditions to which they will be subjected become more demanding. Residual stresses develop because of the mismatch of the thermal and mechanical properties between constituents, affecting the strength and fracture resistance evolved during severe loading. Before a new material can be used in a critical assembly, the evolution of residual stress during service must be accounted for in the predictions of service lifetimes. Because of the complexity of composite systems, computational models that predict the response of the composite are extensively used, but are limited by assumptions concerning the initial and evolving state of the material. Experiments are essential to validate the computed predictions. Neutrons provide the only unambiguous technique that overcomes both of these problems. This research was carried out with support from the Division of Materials Sciences.

Model Improves Understanding of Stress in the Presence of Magnetic Fields

A model has been developed that will be used in evaluating the detection sensitivity of magnetic evaluation techniques which may be developed for nondestructively detecting large stress levels in gas and oil pipelines. This method is important to help ensure that rupture of energy-related structures does not occur.

Dr. M. J. Sablik of the Southwest Research Institute has derived a new expression relating magnetostriction hysteresis to the change of Young's modulus. It has been known that magnetization hysteresis and magnetostriction hysteresis are intrinsically coupled. The current work treats the polycrystalline system as an isotropic system in mechanical equilibrium. Within this approximation, an expression for the magnetostriction was derived as a function of magnetization and of mechanical stress by minimizing the internal energy (including elastic, magnetoelastic, and magnetic terms) with respect to strains. The resulting interaction corresponds to an effective change in the elastic properties of the material, i.e., Young's modulus.

The model predicts that tensile stress tends to open up the magnetostriction hysteresis loop, whereas compressive stress tends to narrow the loop. Also, the interior loops tend to move out more toward the outermost loop as the stress is made more positive. Such effects are also seen in experiments.

Phase Transitions in Buckyball Solids Studied

The free energy of a buckyball (C_{60}) solid has been studied analytically using renormalization group techniques. In particular, the nature of the orientational ordering of the buckyballs has been examined. It is shown that the transition from an uncorrelated orientation of the buckyballs to an oriented structure is strongly driven by fluctuations. The results naturally explain two puzzling experimental observations: (1) a very strong temperature dependence in the free energy as the solid is cooled below the transition temperature; and (2) the strong sensitivity to pressure of the orientational alignment of the buckyballs. A detailed description of the behavior in temperature and pressure around the transition has been derived in terms of the measurements.

While the undoped solid buckyball is relatively mundane, the carrier-doped solid is very fascinating. It becomes superconducting; it has unusual magnetic properties; and it has important mechanical properties, optical properties, etc. Understanding the nature of the orientational fluctuations is an important step to understanding all of these properties and their possible modifications. For example, the conductivity of the doped carriers involve not only phonon scattering, but also the fluctuating orientations of the buckyballs. Magnetic (e.g., magnetic alignment), optical, and mechanical properties will couple to these orientations, resulting in a rich variety of physical phenomena associated with these materials. This research was carried out by Mark Rasolt of Oak Ridge National Laboratory with support from the Division of Materials Sciences.

Dissociation Constants of Oxalic Acid Determined in Saline Solutions

Scientists at Oak Ridge National Laboratory have precisely determined the first and second acid dissociation constants of oxalic acid in dilute to concentrated aqueous sodium chloride solutions to 175 °C using a unique high temperature pH titration apparatus. The effect of salinity is large and significant in modeling the changes in pH of groundwaters and sedimentary basin fluids in which oxalic acid is produced by the decomposition of buried organic matter. The availability of dissociated oxalic acid anion, an important complexing agent for metal ions such as aluminum, actinides, and heavy metals, will be dependent on the pH of the solution, which may be influenced by other environmental parameters. These dissociation constants are critical in the modeling of such processes as groundwater movement, contaminant transport in systems in which oxalate is a significant added component or breakdown product, and enhancement of porosity in hydrocarbon and geothermal reservoirs. In addition, oxalic acid is extensively used in industrial applications and the fundamental data are of broad importance. This research received support from both Geosciences and Chemical Sciences.

New Technique Improves Understanding of Liquid Chromatography

Liquid chromatography is the major separation technique in use today for the analysis of non-volatile compounds. Chemical Sciences researcher Vicky McGuffin, Michigan State University, has reported for the first time pressure effects in solute retention in packed capillary liquid chromatography over the typical pressure range of 1500-5000 psi. Solvent densities vary about 1-5% over these pressure ranges, while solute retention varied from 8-24% depending on the molecule. The magnitude of the increase in solute retention is surprising and could be due to enhanced solvent/solvent interactions with pressure. These new insights, which are based on the development of ultra-sensitive on-column detection in multiple locations on the fused silica, packed capillary column, could lead to a better fundamental understanding of the retention mechanism in liquid chromatography. Further work in this area is underway to better understand the effect of pressure on solute retention.

Cooling History Determined From a Single Grain of Rock

UCLA Professor Mark Harrison, in work funded by the Basic Energy Sciences Geosciences Program, has found a way to determine the cooling history of large terrains by measurements on single crystals of potassium feldspar in common rocks. His method, developed jointly with researchers at the California Institute of Technology and the University of Chicago, features the well-established argon-39/argon-40 technique for determining the age of the rock grain along with careful measurement of the rate of argon loss from the grain at various temperatures. His research was highlighted in a recent issue of Science magazine as potentially important but still controversial. He has applied his new method to rocks from the Bietan plateau with results, consistent with other lines of evidence, showing rapid cooling about 20 million years ago as deeply buried rocks were thrust to the surface.

New Insight Gained on an Important Class of Chemical Reactions

The S_n2 (bimolecular nucleophilic substitution) reaction is one of the most important general class of reactions in chemistry. DOE supported experimental and theoretical work on the S_n2 reaction has been published recently and forms, in part, the basis for interpretation of new experimental results reported in a recent issue of Chemical and Engineering News (C&EN). The theory, including work by Don Truhlar of the University of Minnesota supported by the Chemical Sciences Division, predicts the reaction path proceeds through a double potential minima corresponding to the classical ion-dipole bound complexes which are on either side of an energy barrier that corresponds to the traditional transition state. The theoretical predictions have now been confirmed independently both in highly publicized non-DOE supported studies as well as by examination of isotope effects, considered to be the most sensitive experimental probes of transition-state structure.

Chemical and Engineering News Highlights Materials Sciences/Energy Biosciences Research Efforts

The January 20, 1992, issue of Chemical and Engineering News, the weekly news magazine of the American Chemical Society, contains in the Science/Technology section, two feature articles highlighting recent research accomplishments of two programs supported by Materials Sciences in the Office of Basic Energy Sciences. One, at the University of Illinois, involves the development of a new, in situ transmission electron microscopic technique to study silicon oxidation, an important processing step in the manufacture of semiconductor devices. The technique has made possible the first atomic level observation of the microstructural changes occurring during the processing operation.

The other research project that wa highlighted, supported jointly with Energy Biosciences, at the Lawrence Berkeley Laboratory, involves the development of a general biosynthetic method to insert "unnatural" amino acids and amino acid analogs with modified backbone structures into specific positions in proteins. This research, part of a program to explore the use of biological processes to synthesize new materials, appears likely to have broad applicability for studying factors that affect protein structure-function relationships.

New Methods Developed for Analyzing the High-Temperature Corrosion Chemistry of Aqueous Chloride Ions

New methods have been developed by Chemical Sciences investigators at the Oak Ridge National Laboratory for analyzing corrosion chemistry of chloride ion in high temperature aqueous systems. This is important in various technological systems including power plant steam generators, geothermal energy equipment, deep earth waste repository canisters, and in the formation of ore deposits. Previous methods of analysis were limited to much lower temperatures which could not approximate the actual conditions of corrosion chemistry in high-temperature brines. Both new methods quantify the formation of chemical complexes between metal ions and chloride ions in aqueous solutions up to 250 °C. The first method is based on an innovative silver/silver chloride electrode concentration cell that operates at these elevated temperatures and which directly measures chloride ion concentration. The second method uses a hydrogen electrode which is less direct, but which eliminates the problem in those chemical systems where the metal ion reacts with the silver/silver chloride electrode. At these temperatures the enhanced corrosive effect of aqueous chloride solutions is quantitatively explained by the increasing complexation of metals by chloride ions.

Biogenesis of Methane From Acetate Better Understood

Over the last decade, the metabolic pathway leading to the formation of methane from hydrogen and carbon dioxide has been determined for methanogenic bacteria. The task proved to be very difficult since the enzymes and enzyme cofactors were unique to the pathway starting from H_2 and CO_2. Much of this work had been supported by the Energy Biosciences Program.

Recently, two laboratories supported by the Division of Energy Biosciences have been able to achieve cell-free synthesis of methane from acetate, the first critical step in determining the overall pathway of methane formation from this important substrate. The methanogenic bacteria, Methanoscarcina thermophila and a species of Methanothrix, are being studied at Virginia Tech and Cornell, respectively. The biogenesis of methane from acetate, rather than that from H_2 and CO_2, is believed to be the most prevalent source of biomethane found in nature.

Dynamic Navigation by Robots is Detailed in New Book

A new book entitled, "Motion Planning in Dynamic Environments" by Kikuo Fujimura (ORNL), has been published. The work started as Dr. Fujimura's doctoral thesis at the University of Maryland, and it developed into a full monograph at ORNL's CESAR program supported by the Engineering Research program.

The work departs from past efforts which were limited to robotic navigation in static environments. It is the first book to deal with methods for endowing autonomous intelligent robots with the ability to plan their paths ahead in an environment that may be changing with time.

This research activity is of prime importance for robotics technologies. It not only addresses the problem of collision avoidance with objects crossing the robot's path, but it is also critical for coordinating actions of cooperating intelligent robots under minimal human supervision. This ability is necessary in such contexts as the automated factor, environmental remediation, and space exploration.

New Technique Allows for the Structure Determination of Molecules Adsorbed on Surfaces

An automated low energy electron diffraction (LEED) computational technique has been developed for atomic-scale structure determination of crystalline surfaces from experiment. This technique will allow the direction determination of the structural effects of interactions of atoms and molecules with these surfaces. In one of the first applications of this advanced technique, it was shown that binding of a molecular adsorbate can induce relaxations in a metal surface.

The breakthrough was achieved by a research team led by Michel Van Hove supported by the Division of Materials at Lawrence Berkeley Laboratory and involved the development of an automated search algorithm and the use of "tensor LEED." Tensor LEED is a linear expansion of the diffracted electron amplitudes that is many orders of magnitude faster to compute than competing approaches. The automated search method also permits a very rapid identification of the optimum structural parameters, even when these parameters are numerous. As a result, structures with well over 30 atomic coordinates (x,y,z) can be solved; earlier, far more laborious techniques were limited to five or fewer coordinates.

This advance in the processing of LEED data leaves the dozen competing structural determination techniques far behind. It brings the LEED technique very close to full automation; within the foreseeable future, the experimentalist will no longer need the theoretician's assistance for each and every structure determination. The effect on the field can be likened to the dramatic upswing in X-ray crystallography in the 1960's upon the introduction of direct methods that allowed full automation of bulk structure determination. The technique has already proved its value in the discovery of adsorbate-induced surface modifications, and is likely to have a major impact on the study of heterogeneous catalysis, providing predictive explanations for a variety of previously misunderstood phenomena.

Observation of an Atomic-Scale Grating Structure

For TaC (crystal structure same as that of sodium chloride), it is known that the (100) surface, which consists of alternating chains of carbon and tantalum atoms, has a rippled structure with the C atoms being displaced outward with respect to those of Ta. The ideally terminated (110) surface also consists of C and Ta chains. However, in contrast to the (100) surface, a more complicated structure is observed by low energy electron diffraction (LEED) in which numerous extra reflections between the integral-order beams are observed in these LEED patterns, indicating the presence of a complex unidirectional reconstruction on the [110] surface. Using data obtained from these measurements, a one-dimensional grating-like structural model is proposed, in which the (110) terraces are completely missing. Using this model, an analytical expression to predict the behavior of the diffracted beams has been derived. The average period, L, of the structure is determined to be 6 in units of the surface unit mesh vector length (a = 3.151 Å) along the [110] direction (i.e., a grating with 18 Å periodicity). This unusual surface reconstruction involves multiple missing rows and has not been previously observed.

Atoms in the surface region of a solid usually relax or reconstruct into a structure differing from the bulk in order to minimize the surface-free energy. Generally, reconstructions consist of atomic displacements, missing-row structures, facets, and their combinations. In the past, most investigations have focused on either pure materials or compound semiconductors. Only recently has interest been extended to multicomponent metallic systems. Missing-row structures to date have only involved missing rows in the outermost layer, with a variety of long-range ordered periodic structures. The grating structure found on the surface or TaC(110) has a triangular cross section involving a total of 15 missing rows from the 5 outermost layers. This is the first observation of a periodic structure on a clean low-index surface which requires the displacement of such a relatively large amount of mass. On this surface each atom is missing only one of its nearest neighbors, and appears to be extremely stable and may be the driving force for this novel reconstruction. These results imply that what is known about elemental surfaces of metals is not sufficient to describe and, thus, understand multicomponent alloys. New concepts are needed to explain this unique surface structure. This research was performed by J. K. Zuo, D. M. Zehner, and J. F. Wendelkern, Solid State Division, Oak Ridge National Laboratory, and by H.-N. Yang of Rensselaer Polytechnic Institute.

High Precision Oxygen Isotope Ratio Measurements of Minute Geological Samples Now Possible

Chemical Sciences investigators at Oak Ridge National Laboratory have reported oxygen isotopic ratios, $^{18}O/^{16}O$, at statistical precisions of 1 part per million by secondary ion microscopy analysis of micron-sized inclusions in geological samples. The small spot size and the high precision experimental data obtained from this minute sample, opens a new realm in the analysis of naturally occurring mineral samples.

With this advance, researchers using the ion microscope technique can now rely on secondary ion mass spectrometry to make high precision isotope ratio measurements with 10-20 micron diameter spot sizes from multiple positions on a mineral sample. This is a reduction in required sample size of 10-11 orders of magnitude, without the need for prior sample preparation.

Isotopic variations yield important information about the geological history of the site, the physical history of the mineral sample, and the chemistry of the reactions that occur at the mineral/fluid boundary. These studies will provide a new insight into the transport of hazardous contaminants in soils and groundwater. Small-scale isotopic zonation in minerals can also give information about porosity and permeability in sedimentary basins, which has implications in the exploration for petrochemical reserves.

Mechanism of Sulfur Removal From Thiol Hydrocarbons Resolved

Understanding the removal of heteroatoms, sulfur, in particular, from hydrocarbons has been a long-sought-after goal of researchers in catalysis. A chemist at Oak Ridge National Laboratory has shown that the critical step in the desulfurization reactions, the breaking of the C-S bond, takes place in concert with: a) formation of a C-H bond; b) hydrocarbon desorption; and c) incorporation of the sulfur into the surface. This provides insight into the ultimate sulfur removal step from industrial catalysts. These findings are based on results from a number of surface spectroscopic techniques on a Ni single crystal surface.

Alan Dragoo, Division of Materials Sciences, is Section Chairman for Engineering Handbook on Ceramics and Glass

Dr. Alan L. Dragoo, a project manager in the Division of Materials Sciences, is the Chairman of Section 2 on "Ceramic Powders and Processing," of the recently released ASM Engineering Handbook, Ceramics and Glass. Along with S. G. Malghan, of NIST, Dr. Dragoo also coauthored one of the chapters, "Characterization of Ceramics Powders," in Section 2. The Handbook provides an introduction to the technology for production and characterization of ceramics and glass and to the properties and applications of these materials. Section 2 covers the production, modification and characterization of ceramic precursor powders, beginning with raw materials up to the stage where powders are consolidated into bulk materials.

There has been a growing recognition during the last decade that the powder used in the manufacture of a ceramic material can have a major influence on the quality of the final product. A variety of physical and chemical methods have been developed to produce and manipulate powders to obtain ceramics with desired strength, toughness, electrical properties, etc. Section 2 contains chapters by experts from industry, universities and government laboratories on the variety of methods, and their underlying science, for powder processing and characterization.

Metal Borides Produced by New Polymer-Precursor Syntheses

Metal borides are materials with unique properties including high melting points, high hardness, chemical inertness, and high thermal stabilities, which allow for numerous structural and electronic applications; however, many of these applications require new processible types of precursors which may be used to obtain the borides in film, fiber, coating or shaped-material forms. Work by Professor Sneddon at the University of Pennsylvania is helping to overcome the drawbacks of the classical techniques for forming these interesting materials by efficient, new syntheses involving a polymer approach which has successfully produced two metal borides of particular interest, TiB_2 and ZrB_2.

The new polymer-precursor route has great potential for many technological applications, for example, protection of carbon composite materials from attack by molten metals. Expansion of these studies to other metal borides and non-oxide silicides and nitrides is underway to produce new forms suitable for shaped and coated materials applications.

Interfacial Behavior Observed in Liquid-Gas Flows Using Video Imaging

Professor M. McCready of the University of Notre Dame recently observed and studied the interface of a gas-sheared liquid layer at conditions close to and far from neutral stability. Using a video-imaging system, he was able to observe the mechanism by which the two-dimensional wave field becomes unstable to transverse disturbances. Various wave patterns obtained experimentally agreed well with results obtained from theory. These results are important for predicting behavior in systems with disturbances that occur intermittently in liquid-gas flows such as slug flow and atomization in annular flow.

Water-Based Lubricants Studied Using Unique Apparatus

Several years ago the Engineering Research Program supported a project at NIST for the development of a unique cell using neutron scattering to measure the properties of liquids under high shear. Industry now routinely uses that cell at the NIST neutron beam facility for testing the viability of a new generation of water-based lubricants.

For many applications, it is possible to modify the viscosity of water with additives to make an adequate lubricant, thus replacing oil. However, the usual additives such as polymers are destroyed by high shear, limiting their life-time in applications. Recently, Exxon has devised a means for electrically polarized molecules, the so-called micelles, to arrange themselves into long cylindrical forms, reminiscent of polymers. While these configurations are disrupted by shear, the micelles have the ability to reconstitute themselves to their original polymer-like form. Thus, the molecules retain their effective power to modify the viscosity of water for a long time.

The one-of-a-kind high-shear cell now allows scientists to determine the ultimate limits to which the new lubricants can be pushed with the help of neutron scattering diagnostics.

Novel Uses of Laser Diodes Applied in Analytical Mass Spectrometry

Chemical Sciences investigators at Oak Ridge National Laboratory have reported the use of semiconductor diode lasers for the vapor phase ionization of rubidium with subsequent detection using mass spectrometry. This will enhance the elemental selectivity and flexibility of multiphoton ionization processes.

This technique, known as Resonance Ionization Mass spectrometry (RIMS), gives excellent elemental and isotopic specificity. Semiconductor laser diodes are inexpensive and simple to operate, which makes them attractive for analytical applications. The experiments involved the multiphoton ionization of rubidium using a two diode laser process. This process requires that the two diode lasers be tuned to resonance frequencies for the rubidium atom, which promotes the $5s^1$ ground state electron to an excited 5d level from which it is ionized.

An apparent enhancement in isotopic selectivity was observed during the course of experimentation for the two diode laser process over that seen for a single diode laser scheme. In the future, further use will be made of the narrow-bandwidths, tunability, and spatial coherence of laser diodes in multiphoton ionization.

The Role of Vitamin K_1 in Plant Photosynthesis Elucidated

Vitamin K_1 (2-methyl-3-phytyl-1,4-naphthoquinone) has been identified as the quinone associated with one of two fundamental photochemical centers in green plant photosynthesis. The quinone is a key early link in the electron transport chain involved in the photosynthetic charge separation process. Dr. Marion Thurnauer of Argonne National Laboratory has developed a procedure for replacing this quinone in photosynthetic particles with its predeuterated analog while leaving the protein housing intact. The quinone replacement exchange process was monitored by time-domain electron paramagnetic resonance spectroscopic techniques, which are highly sensitive to deuterium. The quinone function is important in the design of high-yield artificial photosynthetic systems. In addition, the vitamin K_1 pocket may provide a key binding site where new herbicides can attach and interrupt photosynthesis.

Fracturing and Its Effect on Elastic Properties of Brittle Solids Studied

Many currently used models of the behavior of a solid infiltrated by cracks assume a simple relationship between the extent of the damage and the deterioration of the effective elastic stiffness. Recent work supported by the BES-Engineering Research Program carried out by Professor Kachanov (Tufts University) shows that, in general, such a relationship does not exist. The reason for it is that fracture related properties are governed by local fluctuations, while an effective property such as the modules of elasticity is a volume average; that average is relatively insensitive to fluctuations, provided that their density is below a critical value.

The results of this research should have an impact on future models of damage in real structures and on some currently used nondestructive test and evaluation techniques.

Important Coal Liquefaction Reaction Mechanisms Predicted

A new mechanism for the formation of sulfur-sulfur bonds from pairs of sulfur-centered radicals was advanced by researchers at PNL. These results allow the accurate measurement, for the first time, or important reactions of sulfur-containing organic structures which are of importance for understanding coal liquefaction.

Advanced al initio quantum mechanical calculations using supercomputing resources at Florida State University reveal that pairs of sulfur-centered radicals react to form a sulfur-sulfur chemical bond in a triplet excited state which relaxes to the stable singlet ground state disulfide. This knowledge now makes possible the calculation of rate constants for the formation of extremely important disulfide bonds in a variety of chemical and biological systems. For example, thiyl radicals of proteins are predicted to form disulfides at four times the rate previously believed.

These results will significantly aid the understanding of important biological processes, as well as support the potential development of new coal liquefaction processes in which hydrogen transfer and structural reorganization reactions are catalyzed by sulfur.

Effects of Turbulence on Combustion Chemistry Measured

One of the most challenging problems in combustion is the prediction and control of the combined effects of turbulence and chemistry. Until recently, the effects of the interaction between turbulence and chemistry could only be surmised from visualization techniques such as smoke plumes and from deviations of combustion product concentrations from models of combustion reaction kinetics. A series of experiments conducted at the Combustion Research Facility (CRF), Sandia National Laboratories, Livermore, over the past several years has now given us the first evidence of the extent of the influence of turbulence on combustion chemistry. Working with hydrogen-air turbulent flames, CRF scientists have measured every major product and reactant, as well as the molecular radical intermediate, OH, and the temperature as functions of position and time in the flame. At each point in the flame, repeated measurements provide a record of the fluctuation of chemical species and temperature over time. What is observed is significant departure from chemical equilibrium due to large fluctuations in the temperature and mixing fraction of fuel and air. These observations show that combustion is taking place in small, isolated regions where conditions of concentration and temperature allow the reactions to take place. These observations and more to come will provide the kind of detailed data base needed for the development and testing of accurate computer models for the reliable prediction of combustion phenomena.

Atomic Pair Correlations in A Single Crystal Alloy Measured for the First Time

Residual ordering and distances between the atomic species in Ni Fe alloy were measured for the first time by varying the x-ray scattering contrast between Ni and Fe using anomalous x-ray scattering. A synchrotron radiation beamline at the National Synchrotron Light Source at Brookhaven National Laboratory was used to measure the diffuse x-ray scattering from a Ni Fe single crystal. The energy of the x-rays was tuned to enhance or reduce the contrast between the scattering from Ni and Fe. This yielded a result similar to that obtained with neutron scattering but without the need for isotopic replacement, thus, only a single sample was required. Measurements were made with 7.092, 8.0, and 8.313 keV x-rays to allow the Fe-Fe, Ni-Ni and Ni-Fe pair correlation functions to be determined. The method demonstrated by this experiment allowed the determination of the distance between Ni-Ni, Ni-Fe and Fe-Fe pairs in an alloy to be made for the first time. In addition, the enhanced contrast between Ni and Fe increased the precision of the short-range order parameters. The crystal was found to have obvious atomic displacements even though the size difference between Fe and Ni is only 2.5 percent.

Distortions of atomic distances due to differences in size of various atomic species and ordering tendencies between different species are fundamentally important in understanding the mechanical and electronic properties of solid solutions. Prior to this experiment, however, short-range order and atomic distortions could not be measured in materials containing atoms which had nearly the same atomic number except with very time consuming experiments using relatively weak neutron sources. The present experiment is the result of a culmination of efforts in x-ray hardware design and data analysis. In the Ni-Fe alloys, this data will allow a sensitive test of theoretical predictions that magnetism, size differences, and short-range order are coupled. In addition, the method used in this work can be applied to other alloy systems in a systematic search to understand various properties that have been observed but not understood. The measured diffuse scattering can directly test theoretical models of ordering, and the measured short-range order parameters can be used to predict stable low temperature phases.

High Temperature Superconductors Fine-Tuned by Intercalation

Iodine has been successfully intercalated into crystals of all members of the family of Bi-Sr-Ca-Cu-O oxide superconductors by a research group under the direction of Alex Zettl at the Center for Advanced Materials at LBL. The stoichiometry of the 2212 compound was shown to be IBi SrCaCu 0 with the iodine intercalated between the weakly bound Bi-O planes. The c-axis dimension was increased by 7 or 23% while the a- and b-axis dimensions were not significantly affected. The ab-plane of the intercalated 2212 compound shows identical resistivity to the pristine material. The resistance in the c-direction is dramatically altered. Magnetic susceptibility measurements showed a sharp superconducting transition at 80K for a variety of samples, regardless of the T (ranging from 82K to 90K) of the pristine 2212 material. The T of the iodine-intercalated 2223 compound was 100K.

The ability to intercalate iodine into high temperature superconductors opens a door to the engineering of these materials with a view towards increased understanding, control and improvement of their properties. There is a strong possibility that these materials have desirable properties which can be "tuned" by appropriate modification (using intercalates) of the spacings between the lattice planes. Such properties might include T itself, the critical current density in an applied field, or mechanical flexibility of the material. Furthermore, the iodine-intercalated superconductors are stable in air, and the intercalation takes place at relatively low processing temperatures (150 °C) preserving the preformed structures of the host material. The successful intercalation of all members of the family of Bi oxide superconductors (2201, 2212, 2223) suggests that other classes of high temperature superconductors might also be successfully intercalated.

Photoelectron Spectroscopy Developed for Studies on Insulating Catalysts

Chemical Sciences researcher Wayne Goodman from Texas A&M has recently observed for the first time the key molecular vibrational modes of adsorbed molecular methanol on magnesium oxide using high resolution electron energy loss spectroscopy (HREELS). Magnesium oxide is a well-known catalyst support, but detailed studies by electron-based spectroscopies have not been possible due to its insulating properties. The ability to perform photoelectron spectroscopies on insulators opens up the area of surface spectroscopy to the many other insulating types of materials typically used in commercial catalysts. The development of this capability will allow detailed studies on model single crystal catalysts that actually mimic their commercial counterpart.

High Pressure Induces Conductivity in Selected Insulators

A group of researchers led by Peter Yu at the Center for Advanced Materials at the Lawrence Berkeley Laboratory (LBL) have produced an inorganic conducting polymer under high pressure and explained the mechanism for the conductivity. The group has shown that SnI and GeI molecules rotate and become linked through the formation of iodine-iodine bonds under pressures exceeding 7 GPa (about 70 times the atmospheric pressure). This change causes a transformation from a cubic crystalline solid to an amorphous metallic polymeric structure.

In a second experiment, the group applied pressures to materials known as Mott insulators which contain magnetic ions such as Ni, but which are normally insulating. Mott had predicted that if the magnetic ions could be brought close together so that their electronic orbits could overlap, then these materials would become metallic and lose their magnetism. The LBL group found that at pressures exceeding 19 GPa, an antiferromagnetic Mott insulator (NiI), became metallic and nonmagnetic. High pressure X-ray diffraction studies showed the crystal structure to be unchanged from that at atmospheric pressure. Thus, the pressure-induced changes in conductivity and magnetism must result entirely from a change in the electronic structure. These results have been explained qualitatively by Leo Falicov of the LBL theory group using a model based on the interaction of the Ni 3d electrons and the iodine 5p electrons.

New Insights Gained for Methanol Adsorbed on Nickel Surface

A Chemical Sciences researcher, John Yates of the University of Pittsburgh, has observed the first vibrational overtone of the C-O stretch from methanol adsorbed on Ni(111) using single-reflection fast fourier transform infrared spectroscopy. The availability of information from a fundamental vibrational frequency in conjunction with a vibrational overtone from that fundamental frequency provides detailed insight into the nature of the chemical bond. This includes such items as time scales for intramolecular energy transfer and anharmonicities of the bond.

The results from this observation show that the C-O bond is not weakened relative to gas-phase methanol and that the anharmonic shift is decreased by 33%. This result impacts current theories that C-O bond weakening upon adsorption is responsible for the generation of methyl radicals from surfaces.

A New Approach to Non-Equilibrium Thermodynamics

The search for increased efficiency of chemical-to-mechanical energy conversion has led to the need to consider systems with multiple time-asymptotic states - a strictly nonequilibrium situation. Here the conventional techniques of steady-state thermodynamics limited to regions infinitesimally close to stationary states do not suffice. Faced by this new need, Professor J. Ross (Stanford University) and his associates have developed methods for establishing the necessary and sufficient criteria for global stability and relative stability of multiple stationary states. A hybrid free energy, consisting of a combination of Gibbs and Helmholtz free energies has led to the definition of a thermodynamic driving force, or species-specific affinity. Its differentiation yields critical points, and the necessary and sufficient conditions for the stability of steady states. An integral of this affinity provides a valid Liapunov function needed for stability estimates. Physically, that function is related to the work needed to displace the system from a stationary state. It is noteworthy that this approach also yields an extension to far-from-equilibrium of the Einstein equilibrium relation for the probability of fluctuations. Applications to nonautocatalytic and catalytic systems have been published. An incidental result is the discovery of the possibility of multiple stationary states at equilibrium in chemically nonideal systems, such as ionic species. Here it is found that, in principle, chemical oscillations may occur arbitrarily close to chemical equilibrium. That raises doubts as to the applicability of the conventional methods of irreversible thermodynamics. As an example, Onsager's symmetry relations are invalid. These results require rethinking many of the practices and theories in chemical process engineering.

Structural Characterization of Nanocrystalline Pd by X-ray Diffraction Techniques

Scientists from the Los Alamos Neutron Scattering Center (LANSCE) and Argonne have made quantitative X-ray diffraction measurements of ultrafine-grained (nanocrystalline) Pd samples and a coarse-grained polycrystalline reference foil using synchrotron radiation at the National Synchrotron Light Source (NSLS). The intensity profiles of the Bragg reflections from the nanocrystalline samples were considerably better represented by Lorentzian functions than by Gaussian functions, indicating that a large fraction of intensity from the Bragg peaks was found in the tails of the reflections. The remaining intensity differed only slightly for different grain-sized materials; therefore, atomic relaxations in the vicinity of grain boundaries in nanocrystalline Pd must be small in magnitude and/or extremely localized. The results of the present work do not support the previously proposed existence of either a "gas-like" grain boundary phase, or large quantities of vacancies or voids within the grains of nanocrystalline Pd, which produce broadly distributed diffuse scattering. The broadening of the Bragg reflections was related to the small particle size of nanocrystalline Pd and strain located in the grains and/or interfacial regions. Evidence was seen for anisotropic grain shapes preferentially elongated along the [111] direction. The Debye-Waller parameter of nanocrystalline Pd was observed to be larger than the literature value for coarse-grained Pd, which suggests larger displacements of the atoms from their ideal lattice locations in the nanocrystalline material.

Patent Activity in Metallurgy and Ceramics Subprogram at the Ames Laboratory

Three U.S. patents were issued, twelve U.S. patents were pending, six U.S. patents were disclosed, and one foreign patent was pending for the Metallurgy and Ceramics subprogram under the Office of Basic Energy Sciences at the Department of Energy's Ames Laboratory at Iowa State University in FY 1991.

U.S. Patents Issued:

1. "High Strength High Conductivity Cu-Fe Composites Produced by a Powder Compaction/ Mechanical Reduction"
2. "Method of Producing Superconducting Fibers of YBaCuO"
3. "Magnetostrictive Magnetometer"

U.S. Patents Pending:

1. "Electrolytic Capacitor and Large Surface Area Electrode Element Therefor"
2. "Modification of Surface Properties of Cu-Refractory Metal Alloys"
3. "High Strength-High Conductivity Copper Chromium Alloys Produced by Solidification Mechanical Reduction"
4. "Improved Atomizing Nozzle Process"
5. "Strain Tolerant Microfilamentary Superconducting Wire"
6. "Process and Apparatus for Preparing Textured Crystalline Materials Using Anisotropy in the Paramagnetic"
7. "Flame Process for Preparation of Stoichiometric Proportioned Mixed Metal Oxides"
8. "Method for Fabricating Magnets with Partial to Full Volume Loading of Rare Earth-Iron Base Powders"
9. "Rare Earth-Iron Fluoride and Methods for Making and Using Same"
10. "Method for Treating Rare Earth-Transition Metal Scrap"
11. "Rare Earth-Transition Metal Scrap Treatment Method"
12. "Rare Earth-Transition Metal Alloy Scrap Treatment Method"

U.S. Disclosures Submitted:

1. "Transition Metal Grain Refining Precipitates"
2. "High Strength, Light Weight Ti-Y Composites and Method of Making Same"
3. "Pre-Oxygenation of Metal-Quenched Superconductor Oxides"
4. "Rapid Texturing Process of High Temperature Superconductors"
5. "Method for Continuous Preparation of Spherical Forms of Carbon"
6. "High Pressure Gas Atomization of Icosahedral Alloys"

Publication of Workshop on "Hydrogen Interactions with Defects in Crystalline Solids" Helps Identify New Research Opportunities

A paper by the above title that represents the deliberations of a Materials Sciences-organized panel was published in Rev. Mod. Phys., 64, 2, April 1992. It focuses on scientific needs and opportunities. Hydrogen is interstitial and highly mobile in most solids, and it interacts strongly with a wide range of matrix imperfections. Binding energies relative to the solution state extend to about 1 Ev in metals and may reach several Ev in covalent materials and, as a consequence, these interactions remain prominent to hundreds of degrees Celsius. The technological ramifications of this phenomenon include diverse topics such as the potential use of hydride phases to store H fuel; H embrittlement in structural alloys with consequential catastrophic fracture and safety disasters; the passivation of dangling bonds in amorphous Si photovoltaics; various reactions with crystallographic imperfections in single-crystal Si and compound semiconductors; the passivation of interfacial charge traps in SiO grown on Si and the mediation of the radiation sensitivity of devices based on such structures; stabilizing the growth reaction for the synthesis of diamond; and athermal implantation reactions that are a critical issue for the walls of tokomak fusion reactors.

The scientific needs and opportunities that are developed in the paper include point, line, and two-dimensional trapping and reaction mechanisms; H-cluster interaction theory; electronic, effective-medium and band structure theory and methods; cluster modelling; proton quantum mechanics; plastic deformation, cohesion and fracture toughness; H-dopant complexes; deep levels H dimerization; and of course, the compelling need to treat the energetics of the H impurity in a manner closer to first principles and, thereby, to obtain more consistently accurate potentials.

The panel was organized by the Council on Materials Sciences and was chaired by Dr. S. M. Myers of Sandia/Albuquerque. The Materials Sciences liaison to the panel was Dr. Jerry J. Smith. It was the 40th open literature workshop or panel publication since 1980 that focuses on stimulating creative thinking and new ideas in materials research by the Materials Sciences program. The invited participants represented different experimental and theoretical specialties, and had expertise and experience ranging from first-principles fundamentalists to programmatic technologists. As usual, they were selected from the university, private sector industrial, and government laboratory communities. In the present instance there was also a foreign contributor from the Max-Planck-Institut fur Metallforschung.

Basic Energy Sciences Welding Program to be Featured in Reviews of Modern Physics

BES/Materials Sciences-funded investigators, Professor T. DebRoy of Pennsylvania State University and Dr. S. A. David of Oak Ridge National Laboratory, received a request on August 14 by an Associate Editor of Reviews of Modern Physics (RMP) to submit a review article expanding upon their recent review in Science. The RMP editor, Robert W. Keyes, stated that "the interesting and challenging problems that you are discussing there should be brought to the attention of the readers of Reviews of Modern Physics." This is another indication of the growing acceptance of, and interest in, the basic research of welding by the scientific community. Most Federal funding agencies and the scientific community have been slow to recognize the value of and challenges in basic research in welding.

The Basic Energy Sciences welding program is the only Federal program that supports basic research in welding science. It is concerned with the relationship of various parameters involved in the joining of metals and alloys with the microstructure, properties and behavior of weld joints. Since weld failures in fossil, nuclear, and waste storage systems are costly in terms of their adverse safety and environmental impacts as well as system down time, the subject is of critical importance to the NES and the mission of DOE.

Special Report on Supercritical Water Features Work of BES Scientists

In the December 23, 1991, issue of Chemical and Engineering News, a special report appeared on "Supercritical Water - A Medium for Chemistry". Written by an international team of authors, it presents an extensive description of current research on the unique and fascinating properties of supercritical water, including the research programs of a number of BES-supported scientists in universities and the national laboratories. The principal interest for DOE in supercritical water is in its potential use for the safe and effective disposal of toxic wastes. Toxic organic species show dramatically enhanced solubility in supercritical water and their combustion in this environment results in benign, easily treatable wastes.

Supercritical aqueous oxidation is currently under commercial development and has been successfully demonstrated for the treatment of both municipal and industrial wastes. Beyond the potential usefulness for waste disposal, however, the study of the unusual properties of supercritical water, such as its dielectric behavior, viscosity, ionic speciation, and transport, is proving to be a fruitful and stimulating area of basic research.

Technology Transfer

Materials Sciences-Funded Research Helps Spin-off a New Corporation

The American Superconductor Corporation (ASC) of Watertown, Massachusetts, announced a public sale (on December 18, 1991) of 1,670,000 shares of common stock in conjunction with the U.S. Securities and Exchange Commission. Its President and Chief Executive Officer, Dr. Gregory J. Yurek, was the principal investigator for a Materials Sciences grant entitled "Mechanisms of Oxidation of Metals and Alloys" that was initiated in 1985 when he was a professor in the Department of Materials Sciences and Engineering at the Massachusetts Institute of Technology (MIT). By December 1986, it became clear that a new class of high-temperature superconducting materials based upon complex copper oxides had been discovered. In early 1987, Professor Yurek and his coinvestigator at MIT, Professor John Vander Sande, developed a processing technique based upon the oxidation of metallic precursors to produce these superconducting oxides in the form of wire, ribbon or thick-film. Although their invention was made independent of any federal financing, the later development of this technology was directly supported by the Materials Sciences grant, with additional support for this and other technologies coming from NSF. Eventually, Professor Yurek left MIT to assume the position of President and CEO of ASC. Professor Vander Sande assumed the role of principal investigator, and his research on this subject at MIT remains funded by DOE.

The DOE funding was essential in supporting the early research work which expanded on the basic concepts underlying the metallic precursor process and helped develop the technology in its earliest stages. This new area of research involving the metallic precursor approach to producing superconducting wire and ribbon was thereby explored, and the results were made available to the public through 50 publications and 5 patent applications, acknowledged solely to DOE support. This body of work was also available to ASC and was, therefore, instrumental in the process of technology transfer between MIT and industry. Also, Alexander J. Otto, who was supported by the DOE grant while at MIT, completed his doctoral research and joined ASC in October 1991.

Basic Research Leads to Valued Environmental Analysis Technique

Leo Duffy, DOE Assistant Secretary for Environmental Restoration and Waste Management, as the keynote speaker at the Conference (at Erice, Italy) on Innovative Technologies for Cleaning the Environment on April 23, 1992, made reference to "new research and development efforts" which included a field-rugged ion trap/mass spectrometer. He noted that the spectrometer was "developed at ORNL and applied at Savannah River to find TCE (Trichloroethylene) in air, water and soil in essentially real time."

This contribution highlights the role of basic research in addressing the critical environmental challenges facing the U.S. and the world. The development of the ion trap/mass spectrometer at ORNL was predicated on a basic research project supported through the Chemical Sciences Division of BES on ion trap mass spectrometry. The basic research in this project has been described in various BES Highlights, presented to the House Space, Science and Technology Committee in 1989, and to the Office of Management and Budget in 1991. The most recent application of this technique to environmental analysis of volatile organic compounds was demonstrated at Savannah River Laboratory last fall and again this March. In this demonstration it was noted that the technique proved to be much faster than currently accepted methods of analysis and gave excellent agreement with standard EPA methods.

Technique for Sampling Fluids in Deep Drill Holes Developed With Industry

Los Alamos National Laboratory, Drs. Bayhurst and Janecky have recently published details (<u>Drilling Technology</u>, 40, 1992, p. 123-127) on a new high-temperature high-pressure fluid sampler developed in collaboration with Lueutert Instruments. The device is capable of operation at 350 °C and depths of 5 km, in corrosive, particulate-laden, brine environments and provides for retention of dissolved gaseous constituents such that samples representative of the *in situ* environment may be analyzed.

This capability, supported by BES/Geosciences, has been developed to provide fluid sampling capability necessary in the Interagency Continental Scientific Drilling Program and has been tested at the German CSDP site at 3km and in U.S. CSDP drill holes at the Valles Caldera, NM (295 °C), Shady Rest, CA, and Cajon Pass, CA, as well in the International Ocean Drilling Program (hole 504B). Deep, high-temperature oilfield and geothermal brines, important in issues related to energy resource origin and distribution, can be sampled with the new capability.

High quality *in situ* fluid samples are key in providing data for interpreting dynamics of rock-fluid interactions. This success has stimulated additional collaborative efforts in fluid sampling with a goal of further improvements at Sandia National Laboratories, Los Alamos National Laboratory, the U.S. Geological Survey, and scientists participating in the International Ocean Drilling Program.

Space Thermoacoustic Refrigerator (STAR) is Tested Aboard Space Shuttle

A recent flight of the space shuttle Discovery carried a small thermoacoustic refrigerator, built at the U.S. Naval Postgraduate School in Monterey, California, by Steven Garrett and his colleagues. This project is a direct outgrowth of the BES/Division of Materials Sciences-sponsored thermoacoustics work at Los Alamos National Laboratory (LANL) with Gregory Swift and coworkers. Both the invention and most of the basic research behind it were performed by this group at LANL. Garrett was a student at LANL and the STAR is an improved version of the device in his thesis work.

The Tuesday, February 25, 1992, issue of The New York Times contained a long article on the thermoacoustic refrigeration work. The article highlighted the work on a "sonic compressor" which uses sound to compress a refrigerant. The compressor can be substituted for a home refrigerator compressor and can work with new non-CFC refrigerants that won't affect the Earth's ozone layer. The compressor is closely related to the STAR space thermoacoustic refrigerator tested on board the space shuttle. The sonic compressor was developed jointly with physicist Tom Lucas; Lucas holds the U.S. and foreign patents for the compressor. He has formed a company, Sonic Compressor Systems, Inc., to begin commercial development of the system.

The STAR refrigerator uses electric power to drive a loudspeaker, which produces a sound wave in a high pressure helium-xenon gas mixture. Heat exchange elements at the proper locations in the gas enable pumping of a few watts of heat by the sound wave from a low temperature (about -80 °C) to a high temperature (about 25 °C). In this shuttle flight, the refrigerator cooled a heater and thermometer attached to a data recorder. The efficiency of the present refrigerator is about 1/10 of the Carnot efficiency. There is a reasonable chance that further development will bring the cooling power and efficiency to the point where helium thermoacoustics would be a viable alternative to CFC-based vapor-compression refrigeration.

STAR itself is being developed by the Naval Postgraduate School under contract from NASA through General Electric which provides NASA with its life sciences refrigerators. STAR could overcome several known shortcomings in the presently used freon-based refrigerators.

Seven Technology Transfer Awards Given at Lawrence Berkeley Laboratory (LBL)

Seven programs in the Materials Sciences Division at LBL have received ER Technology Transfer Program support awards for Industry-Laboratory collaborations. Negotiations are in progress to establish CRADAs. Each of these projects builds to different degrees on fundamental research supported by the Office of Basic Energy Sciences over the past few years. The projects are collaborations with Motorola (computer display technology), Chemagnetics (Neutron Magnetic Resonance instrumentation), Seagate Magnetics (computer hard disks), Glycomed Corporation (materials for biocompatible structures and devices), DuPont (a new class of helical polymers), Conductus Corporation (superconducting infrared detectors), and IBM (hard carbon coatings).

Computational Materials Science Know-How Transferred to ALCOA

Know-how in the use of computer simulation of interactions of atomic in metals is being transferred to ALCOA by Sandia National Laboratories (SNL) through the Visiting Scientist Program supported by BES/Materials Sciences. Atomistic computer simulation may be used ultimately by ALCOA to provide basic data for the design of both the alloy composition and processing schedule for new commercial alloys of aluminum. Over the last 10 years SNL has developed a highly effective and reliable approach to calculating energy of atoms in metals which takes into account many-body effects and, yet, is computationally fast and easy for the material scientist to use. This approach is called the Embedded Atom Method (EAM) because the energy is calculated for embedding an atom in the sea of electrons provided by the other atoms in the metal. During this decade many material scientists have become acquainted with the EAM through the Visiting Scientist Program.

During the last 3 years, the Visiting Scientist Program has been used to establish effective collaboration with the ALCOA Research Center to assist them in adapting the EAM to a fully dynamic nucleation and growth code. The precipitation of intermetallic and covalent phases is one of the major processing steps in the production of nearly all aluminum alloys, and the development of a predictive capability will form an essential part in intelligent and computer-assisted materials processing at ALCOA. Dr. Robert Hyland of ALCOA has selected the aluminum-scandium system as a model alloy system and has been working with Sandia through the Visiting Scientist Program to apply the EAM to scandium and aluminum.

Fiber Ring Laser Technology Utilized by AT&T

Research by Professor Curtis Menyuk of the University of Maryland on pulse propagation in inhomogeneous optical waveguides has been applied by AT&T to the development of a fiber ring laser that can produce 50 picosecond soliton pulses suitable for long-distance communications. The research by Menyuk was supported by the BES Engineering Program and will be published soon.

Fiber ring lasers using erbium-doped fibers as amplifiers have attracted much attention recently because of their simple structures and the rapid progress in erbium-doped fiber technology. Because erbium-doped fiber amplifiers have a band width of about 30 nm, very short pulses can be generated. In this research, a fiber ring laser proposed by Dr. Linn Mollenauer of AT&T was shown to be greatly improved by adding both a saturable absorber and a frequency limiter so that the laser would mode-lock from initial noise and then remain stable.

This general area of research, soliton propagation in optical fibers, is now generally accepted as the method of choice for transoceanic communication at bit rates exceeding 5 gbits/sec. The recent work by Menyuk has already impacted laser design efforts being carried out by two groups at AT&T, one seeking to produce 50 ps pulsed for long-distance communication applications and another seeking sub-picosecond pulsed for switching and solid-state probing experiments. The simulation codes for pulse propagation in optical fibers developed by Menyuk are also in use by researchers at the Naval Research Laboratory, Harvard, MIT and several other universities.

Improved Infrared Window Materials for Strategic Defense Initiative (SDI) Requirements Derived From BES/Materials Sciences Program

The U.S. Army Strategic Defense Command (USASDC) turned to the Basic Energy Sciences/Materials Sciences (BES-MS) funded program at Oak Ridge National Laboratory (ORNL) for improved infrared window materials required for the SDI program. The USASDC requested ORNL to extend their studies to materials that could be used as infrared windows in the High Endoatmospheric Defense System (HEDS). Using the scientific base and techniques established by the BES-MS studies, the ORNL team developed two routes for increasing the strength and surface smoothness of sapphire windows with little effect on the IR transmission, radiation hardness or laser damage threshold. Under ORNL direction, these procedures were used by industrial companies to produce a full-sized window that is scheduled for flight testing in 1992 by the prime contractor for the HEDS project (McDonnell-Douglas Astronautics Company). Other companies involved were Honeywell, Union Carbide, Ansaco, Laser Power Optics, and Spire. Studies continue to produce and evaluate these and other advanced IR optical materials for SDI applications.

Industrial Support for the Center for Advanced Materials

During Fiscal Years 1991 and 1992 (to date) the Lawrence Berkeley Laboratory's Center for Advanced Materials received $648,000 industrial funding in the form of gifts and work-for-others contracts. Industries providing the support include Dow, Rouge Steel, Mobil, IBM, Union Carbide, Parke-Davis, and Hoeschst Celanese. The Center for Advanced Materials is supported by the Division of Materials Sciences.

Commercial Product Uses High-Temperature Superconductors

One of the first applications of high-temperature superconductors to go on sale was announced at the Materials Research Society Meeting in Boston. Conductus, Inc., of Sunnyvale, California, began selling a complete "superconducting quantum interference device (SQUID)" system in March 1992 for $1,500. The $1,500 will buy the SQUID sensor, the dewar flask to hold the liquid nitrogen needed to cool the magnetometers, an electronics package to interpret the signals, and a user's guide. The SQUID is an extremely sensitive sensor for magnetic fields which has potential applications in geological surveying, nondestructive evaluation of materials, magnetocardiology, and monitoring of brain activity. This is a development from research at the Center for Advanced Materials (CAM) under the direction of John Clarke at the Lawrence Berkeley Laboratory supported by the Office of Basic Energy Sciences. CAM has joined forces with Stanford University, Conductus, Inc., and the State of California as part of its Competitive Technology Program to develop a device for oil field exploration and other applications.

Alcoa Pursues Fundamental Research in Aluminum Alloys At Sandia National Laboratories (SNL)

Alcoa has interest in developing Al-Sc alloys which are stronger than traditional Al alloys. In order to optimize the processing, they want insight into both the diffusion of Sc impurities in Al and into the nucleation rates of Al_3Sc precipitates. Dr. S. Foiles of SNL and Dr. R. Hyland of Alcoa have recently been working together in the development of Embedded Atom Method (EAM) potentials for the Al-Sc system. The EAM, which has proved to be an exceedingly successful atomic level simulation method, has been developed under the Division of Materials Sciences funding. Recently, Dr. Hyland spent 2 weeks at Sandia under the Visiting Scientist Program learning how to use the EAM and developing the potentials. It is worth noting that Alcoa has shown its commitment to developing their own expertise in the area of atomistic simulation by adding a new staff member dedicated to this work.

Cooperative Research Program Underway With Caterpillar, Inc., on Improved Diesel Engines

Caterpillar, Inc., the University of Illinois and others are working together to develop Thick-Thermal-Barrier Coating (TTBC) systems for heat engine applications. Dr. D. Socie of the University of Illinois, who is supported by the Division of Materials Sciences, is a leading expert in the field of material behavior. He will work with Caterpillar design, test, and analysis engineers to develop an understanding of TTBC failure modes, the progression of the TTBC modes from crack initiation to coating spallation, cyclic fatigue behavior of TTBCs, and the interaction between high-cycle and low-cycle fatigue of TTBCs. These findings will be integrated into an analytical life-prediction model which will be tested by Caterpillar in simulated engine environments. This advancement in the understanding of the interrelationships of processing and properties will contribute to the successful development of more-fuel-efficient medium and heavy-duty diesel engines to achieve the goals of industry and DOE.

Ames Laboratory Research Chosen by IBM as "Success Story"

Basic research of BES/Chemical Sciences investigator, Marc Porter, on the study of fluorinated monomolecular assemblies and the interaction between these self-assembled monolayers and metal surfaces has been spun-off into a research contract with IBM. The research effort has been so successful that it has been cited as one of IBM's research contract "success stories." This is another good example of technology transfer between basic research supported at the national laboratories and industry. Porter's research has impacted present and future products at IBM in the microelectronics packaging segment of their business. The specific products under consideration are looked upon as proprietary information by IBM and details are not currently available. His work with IBM is cited as a positive fostering of relationships between IBM and Iowa State University (Ames Laboratory).

These monolayers mimic polymer interactions with metal surfaces. The understanding of the chemistry and structure of the polymer/metal interfacial region is important in the study of adhesion. IBM's interest involves the understanding of metal/polymer adhesion and the deterrence of delamination which aids in alternate designs or processes in microelectronics packaging.

Seven BES-Supported Projects Honored With 1991 R&D 100 Awards

DOE facilities-based research won 36 of 100 awards from R&D Magazine for 1991. Two projects at Ames Laboratory, two at Lawrence Livermore, one at Argonne and one at Brookhaven were directly supported by BES programs. In addition, one BES-supported research effort not affiliated with a national laboratory also won an R&D 100 award. The seven awardees are:

Argonne National Laboratory - Strontium-Specific Resins Developed for Radionuclide Chromatography

Traditional methods for this separation and preconcentration suffer from a number of drawbacks, in particular, complexity and ineffectiveness with highly acidic sample solutions. To overcome these problems, Dr. E. Philip Horwitz and Mark L. Dietz from Argonne National Laboratory have developed a series of novel extraction chromatographic resins, referred to as the Spec™ resins, capable of selectively removing one or more metal ions from aqueous solution. Each of these resins combines a highly selective metal ion extractant (either alone or in combination with a suitable organic solvent) with an inert polymeric support. The result is a solid sorbent pairing the selectivity of liquid-liquid extraction with the convenience and ease of handling of an ion exchange resin. This strontium-specific resin could be used in a variety of applications, ranging from strontium determination in soil and water to quality control in radiopharmaceutical agents. Dr. Horwitz received an R&D 100 award in 1987 for his development of the TRUEX separation process.

Ames Laboratory - Microfluor Detector Commercialized

Dr. Edward S. Yeung developed the "Microfluor" fluorescence detector for capillary separation techniques. The Microfluor detector can precisely analyze very small amounts of a material, helping scientists who want to study substances that are limited in availability, such as the chemicals in a single living cell or an expensive new drug. Scientists at Ames Laboratory predict that the detector will provide crucial support in projects on the forefront of medicine, biology and materials chemistry. The detector, the first commercially available unit of its kind, irradiates samples with a laser beam instead of a conventional light source. Many important chemical and biological substances give off light or fluoresce in the presence of a laser. Others can be made to fluoresce. The detector analyzes this light to measure the presence of a substance. As a result of this and other improvements, it can analyze with high sensitivity samples 50 times smaller than those required by other detectors. Other advantages include the ease with which the Microfluor detector can be used; the detector's cost-effective design; and its ability to operate in a fully lighted room.

Ames Laboratory - High Pressure Gas Atomization Technique Employed to Create Rare-Earth Permanent Magnet Alloys

The Ames Laboratory developed a high pressure gas atomization technique for making rare-earth iron permanent magnet powder. It uses a unique supersonic nozzle and a novel atomization chamber to produce ultrafine powders of high performance permanent magnet alloys. A key advantage of the Ames powder is a protective surface film that is applied by a gas phase reaction during atomization. The Ames powder also has a consistently fine, spherical shape which is well suited for fabrication either of conventional sintered magnets or of magnets made by complex shape forming processes like metal injection modeling and hot isostatic pressing.

Major improvements in electric motor efficiency would lead to a major reduction in energy consumption. The use of high flux density Nd-Fe-B magnets in motor construction could save 0.3 Quad annually by allowing downsizing of motors. The Ames magnet powder production approach allows the safe, energy-efficient, and cost-effective manufacturing of high performance Nd-Fe-B magnets to permit this material to realize its full range of potential applications. Two principal applications of these magnets that are enabled by the Ames powder process are in the fields of automated motion and computers, for example, energy efficient automobiles (e.g. large, high torque D.C. servo motors) and automated motion (e.g., precision stepper motors for disk drives and robotics).

Brookhaven National Laboratory - High Resolution Scanning Photoelectron Microscope Developed

An Industrial Research Magazine R&D 100 Award was given to a group of researchers from SUNY-Stony Brook, Brookhaven National Laboratory, the Center for X-ray Optics at Lawrence Berkeley Laboratory, and IBM for the development of a high resolution scanning photoelectron X-ray microscope which uses radiation from a soft X-ray undulator beamline at the National Synchrotron Light Source at Brookhaven. This microscope can identify features as small as 0.1 micrometers, and by tuning the X-ray wavelength with a monochromator, can provide element-sensitive images on this scale. The brightness of the undulator source, together with the advanced optics, makes possible the successful operation of this instrument. The microscope uses a Fresnel zone plate to provide a finely focussed beam of X-rays which is scanned across the sample, and uses a grating monochromator to select photon energies which will selectively excite different elemental species in the 400 to 800 electron volt range. The microscope can be used to examine microstructural features of materials, including the distribution of different chemical species in a sample; the structural features of a lithographically engineered microcircuit, as well as features of biological materials such as cell nuclei, all on a scale of less than one micrometer.

Lawrence Livermore National Laboratory (LLNL) - Stanford Synchrotron Radiation Laboratory Used to Develop Tomographic Microscope

An R&D 100 Award was made to a team of researchers at the LLNL who have developed an X-ray tomographic microscope which provides a 3-dimensional view of the interior of a material sample. The new microscope uses the principles of computerized axial tomography (CAT) scanners that are used for medical diagnosis, and requires a source of extremely parallel X-rays such as that provided by the 31 pole wiggler source at the Stanford Synchrotron Radiation Laboratory. In materials research, X-ray tomography yields information about the nature and distribution of structural defects or damage within the interior of materials. X-rays are used to look at a sample nondestructively. There is no need to provide ultra-thin samples or specially treated surfaces in order to get the 3-dimensional image. The X-ray tomographic microscope has been used to study such diverse materials as teeth, laser fusion targets, and metal matrix composites (materials with embedded, strength-enhancing fibers). Laboratory scientists have been able to observe, in situ, the shape of cracks formed when such composites are under stress.

Lawrence Livermore National Laboratory - Discovery of Unique Laser Materials Enable the Development of New Laser Systems

A research team at LLNL discovered and developed a class of new laser materials that have many potential DOE, DOD, and industrial applications. The discovery of these materials was guided by insight and search criteria obtained several years earlier from BES-supported basic research by Stephen Payne and Lloyd Chase and collaborators on excited state absorption mechanisms of the Cr^{3+} ion and the isoelectronic V^{2+} ion in various crystalline hosts. The new materials, $LiCaAlF_6$, $LiSrAlF_6$, and $LiSrGaF_6$ doped with chromium ions, have an unprecedented combination of optical, physical, and crystal growth properties that make them highly attractive as tunable Cr^{3+} lasers and amplifiers. These lasers are currently being used in the Inertial Confinement Fusion Program at LLNL to amplify subpicosecond pulses to extremely high peak powers for plasma physics research and for other applications. Several laser companies and industrial laboratories are licensed by LLNL to develop these lasers for a variety of DOD and scientific applications.

Jet Process Corporation - Process Deposits Thin Films From Vapor

A nonfacilities-based BES-supported research effort by the Jet Process Corporation (formerly Schmitt Technology Associates) has also received an R&D 100 Award for its Jet Vapor Deposition (JVD) process. JVD is a new process for producing uniform, high-quality thin films and ultrafine particles at high rates, at low temperature, and in low vacuum. JVD can deposit thin films of a wide variety of metals, oxides, nitrides, semiconductors, organics, and compounds. It can be used to coat wires, tapes, fibers, and inside channels and tubes.

The JVD process uses a nozzle to produce a supersonic stream of inert carrier gas. The material to be deposited is seeded into the carrier gas from a source positioned within the nozzle. Following nozzle expansion, the composite vapor is transported to the surface of the substrate, where it deposits to form a hard, dense adherent coating. The basic process, which has been patented by Jet Process Corporation, was developed during 1987-90 with support from the BES-Division of Advanced Energy Projects. The corporation has received an order to coat 20,000 ceramic wafers with a thin film of copper/gold using this process.

Cooperative Research and Development Agreements

At present, over 98 Cooperative Research and Development Agreements (CRADAs) have been signed or are in negotiation between DOE national laboratories and U.S. industry which stem from BES-supported work at the laboratories. Presented below are seven such CRADAs which have been recently signed.

Los Alamos National Laboratory/Tektronix, Inc., Signs CRADA on New Refrigeration Technology

Los Alamos National Laboratory and Tektronix, Inc. have now signed a CRADA, using funds from the Advanced Industrial Concepts Division, Conservation and Renewable Energy as the DOE contribution, to develop and miniaturize the thermoacoustically driven pulse-tube refrigerator (a.k.a. Coolahoop) for cooling superconducting electronics. This refrigerator, like the Space Thermoacoustic Refrigerator (STAR) under development for space applications, uses sound and a nonchlorofluorocarbon refrigerant to produce cooling. The invention of this type of refrigerator and the technology base work on the underlying principles was performed under support from the Office of Basic Energy Sciences, Division of Materials Sciences. Dr. Gregory W. Swift of Los Alamos National Laboratory is one of the inventors and the principal investigator on the work. Los Alamos National Laboratory signed the CRADA on July 10, 1992. Tektronix, Inc., signed the CRADA on August 11, 1992.

CRADA on Superconducting Materials Continues Between Oak Ridge National Laboratory and IBM

A CRADA between Oak Ridge National Laboratory (ORNL) and IBM Corporation has been extended. The agreement covers research to study magnetic flux motion and pinning in high temperature superconductors (HTSCs) making use of the facilities and expertise of both ORNL and the Thomas J. Watson Research Center of IBM.

In the first year of this project, proton irradiation was used to increase the critical current (J_c) of YBaCuO single crystals. Due to the very small superconducting coherence length in this HTSC, these defects act as effective pinning centers. The proton irradiation contributed randomly distributed point defects which acted as pinning centers and resulted in large enhancements in J_c. However, it became clear that each defect could pin only a small portion of the core of a vortex. The critical current could be enhanced by increasing the density of these defects, but only to the point where the defects are approximately one coherence length apart.

To overcome this limitation, it was necessary to introduce a different shape of defects. The optimal pinning sites consist of long columns on nonsuperconducting materials each of which is capable of pinning a long portion of a vortex core. This was done by irradiation of superconducting single crystals with very energetic heavy ions (580 MeV Sn^{30+}) at the Holifield Accelerator Facility at ORNL to create long tracks of defects in the superconductor. This resulted in a much higher critical current (7 x 10^4 Amp/cm^2) at high temperature (77K) and high magnetic fields (5 Tesla) when the magnetic field is aligned with the columnar defects.

Work will continue for another year under the CRADA, looking at a variety of HTSC materials, and using a variety of irradiation species, such as 2 GeV Au ions. The CRADA is in effect from February 1, 1992, through January 31, 1993.

Biomimetic Coating CRADA Between Pacific Northwest Laboratory and AC Rochester

The concept of mimicking the principles of biological hard tissue formation to make engineering-useful materials was developed at Pacific Northwest Laboratory (PNL) originally on the program, "Ceramic Composite Synthesis Utilizing Biological Processes," which is funded by DOE's Office of Basic Energy Sciences/Division of Materials Sciences. This program, guided by Drs. Peter C. Rieke and Bruce C. Bunker, developed the fundamental understanding necessary to produce ceramic coatings such as Al_2O_3 or Fe_2O_3 on polymer, ceramic, or metal surfaces from a low-temperature aqueous solution. Since this process offered the potential to produce inexpensive hard coatings on complex shapes while producing no hazardous wastes, DOE-Conservation Energy Office of Industrial Technology funded the adaptation of this process to industrial needs.

The "biomimetic" process adapted to industrial use quite nicely since it could easily and inexpensively put hard coatings onto complex shapes of metal and plastic parts. This allowed lighter-weight materials with a hard coating to be substituted for heavier materials, thus allowing parts to last longer.

Carl Miller, AC Rochester (Flint, MI), was introduced to the "biomimetic" coating technology during a tour of PNL. He became convinced that this process was exactly what was needed to solve current materials problems in the automobile fuel delivery system. A visit to AC Rochester by Dr. Gary L. McVay, PNL, resulted in a CRADA being written to develop hard coatings for fuel delivery systems, which was signed by GM/AC Rochester on May 18, 1992, and by PNL on May 19, 1992. The coatings serve as both corrosion protection and wear-resistance enhancement, and they can be applied to the complex shapes of metal and plastic fuel pump parts. Additionally, the coatings can be used on the inside surfaces of high-density polyethylene fuel tanks to reduce permeation emissions through the tank. Corrosion problems are particularly important for alcohol-containing fuels.

PNL's role is to adapt the "biomimetic" process to the specific needs of AC Rochester. The role of AC Rochester is to supply the parts and evaluate the coatings. PNL received a funding level of $300K/year from DOE-CE's Office of Industrial Programs; AC Rochester also is spending $300K/year in-house. This activity is scheduled for 3 years and will expand to other automotive components. Currently, there is a regular exchange of staff between PNL and AC Rochester as processes move toward production scale-up.

The "biomimetic" approach to industrial hard coatings offers numerous advantages. PNL is now discussing applications with General Motors as well as the 3M Company. As environmental regulations increase, the "biomimetic" process becomes increasingly more appealing to industry. This is a perfect example of how an idea was developed by DOE-BES, picked up by DOE-CE (applied research), and spun off to industry.

Oak Ridge National Laboratory Implements CRADA with EPRI

Oak Ridge National Laboratory (ORNL) has implemented a CRADA with the Electric Power Research Institute (EPRI) on advanced deposition and substrate technologies for thin-film polycrystalline silicon. The agreement, jointly funded by EPRI and Energy Research, builds on expertise at ORNL in the areas of thin-film processing and ceramics and was developed in research programs supported by Basic Energy Sciences/Division of Materials Sciences. The CRADA involves close cooperation between EPRI and the Solid State and Metals and Ceramics Divisions at ORNL to develop new approaches to the large-scale deposition of polycrystalline silicon onto low-cost substrates for the fabrication of high-efficiency, cost-effective solar cells for photovoltaic conversion of solar energy.

Ceramics CRADA Signed Between SNL and Dow-Corning Corporation

A CRADA has been signed between Sandia National Laboratories (SNL) and Dow-Corning Corporation to develop new processing methods for silica-filled siloxane elastomer composites. These strong elastic materials are used in building materials, seals and electrical cables. Dow-Corning contacted Sandia because of its Materials Sciences-funded ceramics work on solution polymerized silicates in which SNL used small angle neutron scattering and fractal concepts to elucidate the structure of branched silicate macromolecules. SNL and DOW-Corning will demonstrate in situ chemical methods as a new route to composite materials in which chemical rather than mechanical mixing methods are used. The joint research seeks to tailor the structure of the glass silica filler phase to optimize properties for particular applications. The proposed research will closely track the approach taken in the BES ceramics program.

Initial research demonstrated that a key factor (proprietary under the CRADA agreement) controls the size scale of the phase-separated domains. Work is now focusing on the control of the interface between the glassy and rubbery phases.

The Defense Programs Technology Commercialization Initiative (TCI) funds SNL's contribution at $250K/year. Dow-Corning is matching this support with in-house research. SNL and Dow-Corning share responsibility for synthesis. SNL, Dow-Corning, the University of Cincinnati and the University of New Mexico provide mechanical and structural characterization. Prior to TCI approval, the project began with BES funds from the Center of Excellence on Synthesis and Processing.

Sandia scientist, Tamara A. Ulibarri spent 2 weeks at Dow-Corning's Midland, Michigan, laboratory learning proprietary synthetic methods.

Ceramics CRADA Signed Between ANL and Allied Signal, Inc.

A new CRADA has been signed by Allied Signal, Inc., and Argonne National Laboratory (ANL) for further investigation of the resistance of the ceramic silicon nitride (Si_3N_4) to fracture and particulate erosion damage. This CRADA activity is in follow-up to earlier Materials Sciences-funded fracture and erosion studies carried out by Dr. Jules L. Routbort at ANL, and will now focus on how cracks originate and grow in Si_3N_4 under applied stress and erosive conditions, and how such crack behavior is affected by different fabrication techniques. Allied Signal will provide samples of two types of Si_3N_4 to ANL and will measure their resistance to the nucleation and growth of cracks. ANL will perform experiments to measure erosion and develop theoretical models to quantitatively predict cumulative erosion damage under the direction of Dr. Routbort. The project is to last for 12 months and will be funded with $50,000 from both ANL and Allied Signal, Inc.

CRADA for the Evaluation of Corrosion Established Between BNL and Basic Aircraft Research (BAR)

The Brookhaven National Laboratory (BNL) Corrosion Group under the direction of H. S. Isaacs with the support of BES-Materials Sciences, has over a number of years pioneered the use of the Scanning Vibrating Probe (SVP) to study current distributions on corroding surfaces in wet environments. The surface is also viewed with a microscope so the current distribution can be correlated with microstructural features on the metal surface. The SVP technique is particularly well suited to the study of corrosion inhibitors. The advantages of this technique for studying corrosion inhibitors became apparent to Mr. R. Maldonado, of Basic Aircraft Research. He contacted Dr. Isaacs who agreed to help him to apply basic corrosion techniques, as well as the SVP. The BNL Corrosion Group wrote a proposal "Corrosion Inhibitors for Aircraft" for an Industry-Laboratory Personnel Exchange which was funded by the Laboratory Management Division, Office of Energy Research, initially at a level of $35K which was then increased to $50K. The proposed work involved using the unique capabilities of the SVP at PNL and the experience of the PNL Corrosion Group to assist Mr. Maldonado in elucidating the mechanism of corrosion resistance of compounds currently in use. Evaluating the performance of alternative compounds with a long-term view of finding better inhibitors and developing criteria for Federal Aviation Administration approval of the use of these compounds is also a goal. Recently, BAR and BNL have signed a CRADA for this work. The importance of the SVP to the collaborative effort was recognized and provisions for its use were written into the CRADA.

Small Business Innovation Research (SBIR)

Phase I Awards Selected

The Department of Energy received 1,534 applications in response to its tenth SBIR solicitation, which contained 35 technical topics, by the closing date of January 27, 1992. This is the third largest total in the program's history. The most popular topic was Materials Sciences in BES with 144 applications. Another BES topic, Chemical Sciences Research, received 90 applications. The Phase I award selection was completed on schedule for the tenth consecutive year. A record number of 202 projects were chosen for awards. The Phase I grants are for about $50,000 over a period of about 6 months, and will begin on July 27, 1992. The technical topic areas in ER with the most awards are Technology for the Superconducting Super Collider (15), Chemical Sciences Research (14), Technology and Instrumentation for High Energy Accelerators (14), and Materials Sciences (10). Secretary Watkins announced the award selection in the San Francisco area on May 27, 1992.

Presentation Given at the Spring American Physical Society Meeting

Dr. Samuel Barish presented an invited paper in a session entitled "Entrepreneurial Physics" at the Spring Meeting of the American Physical Society on April 21, 1992, in Washington, D.C. In his presentation, Dr. Barish described the SBIR program in all Federal agencies. He also explained how physicists could start their own companies by winning SBIR grants, with the eventual goal of commercializing products and processes.

Commercialization Assistance Project (CAP) Success

As a result of participating in the DOE SBIR Commercialization Assistance Project (CAP), ADA Instruments, Inc., of Englewood, CO, has signed a licensing agreement with Land Combustion of Bristol, PA. Under the agreement, Land Combustion will commercialize the ADA Multigas Analyzer developed with DOE SBIR funds. The estimated income from the royalties is $1.2 million over the next 3 to 5 years. The analyzer, originally developed for measuring NH_3 in flue gas using a photodiode array with unique software, has been extended to measure NO and SO_2 as well. ADA has stated that participation in the CAP was the key to making the agreement happen. DOE is the only agency that conducts such a project as the CAP, which provides individual assistance in business plan development.

Reauthorization Bill Introduced

On March 5, 1992, H.R. 4400 was introduced and referred to the House Small Business Committee. This bill would extend the SBIR program from October 1, 1993 to October 1, 2000. It would increase the set-aside for SBIR from 1.25% of the extramural research or R&D budget of Federal agencies to 2.5%. The increase would begin in FY 1994, with increments of 0.25% per year, and would reach 2.5% in FY 1998. H.R. 4400 would also increase the maximum size of Phase I awards from $50,000 to $75,000, and would give much more weight to commercialization potential in the evaluation of Phase II grant applications. Congressional hearings on the bill are in process.

Meeting With Congressional Staffer Held

At the request of Mr. Russell Orban, Staff Director of the Subcommittee on Procurement, Tourism and Rural Development of the House Small Business Committee, a meeting was held on February 7, 1992, to discuss the SBIR program. Mr. Orban is currently drafting legislation on the reauthorization of the SBIR program, which is scheduled to end on October 1, 1993. Dr. Samuel Barish, Dr. Walter Polanskỳ, and Mr. Frederick Tathwell (Office of Congressional and Intergovernmental Affairs) attended the meeting. Mr. Orban asked for the meeting to further discuss two subjects presented by Dr. Barish at an interagency SBIR Program Managers meeting on January 28: (1) the DOE system of providing continuous funding between Phases I and II; and (2) the emphasis on commercialization of SBIR research in the operation of the DOE program.

Inc. Magazine Recognizes SBIR Awardees

Five DOE SBIR awardees were chosen among the 500 fastest-growing American private companies, in the December 1991 issue of Inc. Magazine. The SBIR firms and their areas of research are: ACCSys Technology, Inc., Pleasanton, CA - linear accelerator technology; ADA Technologies, Inc., Englewood, CO - peroxy and ammonia detectors for fossil energy research; PAI Corporation, Oak Ridge, TN - space nuclear power and coal liquefaction research; Physical Optics Corporation, Torrance, CA - fiber optics and holography; and Synetics Corporation, Reading, MA - high energy physics data processing. The 500 companies were chosen, out of 21,000 candidates, on the basic of percentage growth in sales from 1986 to 1990. The SBIR effort was partly responsible for the sales growth of the five firms, which ranged from 1025 to 3030 per cent. During this period, the companies increased their number of employees by an average factor of 15.

Congressional Testimony Given

Dr. Samuel Barish presented testimony on the DOE SBIR program before the Subcommittee on Procurement, Tourism, and Rural Development of the House Small Business Committee on November 26, 1991. DOE was one of four agencies that testified, out of the eleven agencies with SBIR programs to testify. The testimony was well received by the Subcommittee, and DOE was especially praised for success in providing continuity of funding between Phases I and II for 8 consecutive years. As a result of the hearing, the Department may receive questions on policy issues from the Subcommittee. The hearing was one of several held this Fall in preparation for legislation on the possible reauthorization of the program, which is scheduled to end on October 1, 1993.

SBIR Awardee Wins Clean Coal IV Contract

As a follow-on to a 1985 SBIR Phase II project ($492 K), ThermoChem, Inc., of Columbia, MD, has been chosen for a $37.3 M award in the Department's fourth round of the Clean Coal Technology Program. The project, entitled "Demonstration of Pulse Combustion in an Application for Steam Gasification of Coal," will be funded by DOE (50%) and by Weyerhauser Paper Company and others. The gasification process will produce a medium Btu-content fuel gas from subbituminous coal at Weyerhauser's mill in Springfield, OR. The objective of ThermoChem's project is to convert over 400 tons of coal per day to gas and steam. The technology also has the potential for widespread applications in the paper industry and could be used to supply the gas needs of other industries, as well as those of electric utilities.

SBIR Completes Negotiations With Walcoff and Associates, Inc., for Support Work

The Contracts Division at the DOE Chicago Field Office has completed negotiations for a new contract with Walcoff and Associates, Inc., an 8A firm located in Alexandria, VA, for work to support the SBIR program which began September 2, 1991. The contract is a 5-year contract totalling $1,509,474.52. The base year is for $262,661.15; year two for $282,610.01; year three for $303,033.17; year four for $321,054.55; and year five for $340,115.64. This allows Walcoff to continue the good support they have provided to SBIR for the past 3 years.

Awards and Recognitions

1993 American Chemical Society National Awards Announced

It was announced that eleven investigators funded by the Office of Basic Energy Sciences were chosen to receive national awards for 1993 from the American Chemical Society. These awards include Colloid or Surface Chemistry to D. Wayne Goodman of Texas A & M University, Inorganic Chemistry to Gregory Kubas of the Los Alamos National Laboratory, Organometallic Chemistry to Robert H. Crabtree of Yale University, Petroleum Chemistry to Bruce C. Gates of the University of Delaware, the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry to David M. Hercules of the University of Pittsburgh, the Peter Debye Award in Physical Chemistry to F. Sherwood Rowland of the University of California, Irvine, the Chemistry of Materials Award to Rustrum Roy of Pennsylvania State University, Distinguished Service in the Advancement of Inorganic Chemistry to Theodore L. Brown of the University of Illinois, MRL, an Arthur C. Cope Scholar Award to Peter Chen of Harvard University, and the Noble Laureate Signature Award for Graduate Education in Chemistry to Sylvia T. Ceyer of the Massachusetts Institute of Technology. Argonne National Laboratory investigator E. Philip Horwitz received the Glenn T. Seaborg Actinide Separation Special Recognition Award for the development of separations chemistry important to nuclear waste management. Lawrence Berkeley Laboratory investigator Alexis T. Bell received the Langmuir Lectureship of the Division of Colloid and Surface Chemistry.

Arthur L. Schawlow Prize Will be Presented to Yuen-Ron Shen

The 1992 Arthur L. Schawlow Prize will be presented to Professor Yuen-Ron Shen (University of California at Berkeley) during the International Laser Science (ILS-VIII) meeting, September 20-24 in Albuquerque, New Mexico. Established in 1991 and sponsored by the NEC Corporation, the purpose of the prize is to recognize outstanding contributions to basic research that uses lasers to advance the knowledge of the fundamental physical properties of materials and their interaction with light. Born in Shanghai, China, Professor Shen received his Ph.D. from Harvard University in 1963, and spent the following year as a post-doctoral fellow at the same institution. He joined the faculty of the University of California at Berkeley in 1964, where he is presently a professor of physics. Professor Shen's research in nonlinear optics established the foundations for the study of both liquid crystals and interfaces, and subsequently led to important device applications. His citation reads, "For his seminal contributions to nonlinear optics and spectroscopy, in particular for his discoveries of structural properties of surfaces, interfaces, and liquid crystals through their second order optical responses." Professor Shen has been supported for many years by the Division of Materials Sciences at the Lawrence Berkeley Laboratory.

Chemical Sciences Grantee Receives Top British Award

University of Georgia Professor Henry F. Schaefer III has been named to receive the 1992 Centenary Medal of the Royal Society of Chemistry for his work in computational quantum chemistry. Professor Schaefer has been supported by the Chemical Sciences Division, initially at the Lawrence Berkeley Laboratory, and now at the University of Georgia. He has distinguished himself throughout his career by addressing fundamental questions in chemistry of interest to experimentalists and theoreticians alike. He was one of the first of an emerging breed of quantum chemists who believe their theoretical predictions of molecular structures and energies can be more reliable than experimental values. His first great success in this area was in 1970 with the determination of the molecular structure of the important combustion intermediate CH_2. The structure, as determined spectroscopically by Nobel Laureate Gerhard Herzberg, was determined to be linear, an experimental finding that was widely accepted. At the time Schaefer published, it was unheard of to suggest that a result from quantum chemistry calculations could be more reliable than one determined by experiment, let alone by an experiment performed by such a renowned spectroscopist as Herzberg. Schaefer's insistence that the CH_2 molecule was bent was eventually borne out by experiment. Since then Schaefer has been a major contributor to our knowledge of the structures and energies of free radicals and their reactions.

Geochemists Receive Honorary Degrees From the University of Chicago

Two outstanding researchers who have been supported by the BES program received honorary D.Sc. degrees from the University of Chicago recently. Harmon Craig, Scripps Institution of Oceanography, University of California at San Diego, was supported during 1984-1988 and Gerald Wasserburg, California Institute of Technology, has been continuously supported since 1988. Both researchers were cited for their contributions in isotope geochemistry.

Lawrence Berkeley Laboratory Materials Scientist Honored with a Rare International Award

Dr. Robert O. Ritchie, Director of the Center for Advanced Materials at the Lawrence Berkeley Laboratory, has been awarded the 1992 Rosenhain Metal by the Institute of Materials (London, U.K.). This prestigious international honor is awarded to no more than one scientist per year. The citation to Dr. Ritchie states "...in recognition of distinguished achievement in metallurgy and materials science...." The award ceremony took place in London in May 1992. Another previous American winner of this award is Professor Gareth Thomas, also of the Lawrence Berkeley Laboratory.

Acta Metallurgica Gold Medal Awarded to Professor Jerome B. Cohen

Professor Jerome B. Cohen of Northwestern University in Evanston, Illinois was awarded the 1992 Acta Metallurgica Gold Medal at the Minerals, Metals and Materials Society Annual Meeting held March 1-5, 1992, in San Diego, California. The Acta Metallurgica Gold Medal is awarded annually in recognition of outstanding ability and leadership in materials research. Professor Cohen's research is supported by the Division of Materials Sciences, Office of Basic Energy Sciences.

BES-Supported Chemists Are Among the World's Most Cited

"Science Watch," a publication of the Institute for Scientific Information (Current Contents) that tracks trends and performance in basic research has recently published a list of "The World's Most Cited Chemists Ranked by Total Citations, 1984-1991". The data is based upon publications that have appeared in any of 339 chemistry journals between 1984-1990 and citations to these papers through the end of 1991. Of the top 50, 40 are U.S. scientists and 16 of those are supported by Basic Energy Sciences. When the extraordinary broad range of research interests in Chemistry is considered, it is noteworthy that over one-third are supported by BES; and it is another indicator of the high quality of the BES-supported scientists and the peer acceptance of their work.

Curie Medal Awarded to Chemical Sciences Investigator

Robert H. Schuler, Director of the Notre Dame Radiation Laboratory, was recently awarded the Maria Sklodowska-Curie Medal by the Polish Association of Radiation Research in an award ceremony in Cracow. The award, presented in commemoration of Madame Curie who was born in Poland, is given to prominent scientists involved in radiation chemistry or radiobiology research. The first Curie Medal was awarded in 1983 to Lord Frederick Dainton, Chancellor of the University of Sheffield. Professor Schuler is the thirteenth recipient, and the first American, to receive the award.

Energy Biosciences-Supported Biologist Receives MacArthur Fellowship

Professor Sharon R. Long of the Department of Biological Sciences, Stanford University, was named a recipient of a fellowship from the MacArthur Foundation of Chicago. She was one of 33 people announced on June 15, 1992, to receive the annual awards. The John D. and Catherine T. MacArthur Foundation created the fellowships in 1981, with the objective of freeing "exceptionally gifted individuals" from economic constraints so they could develop their potential. Dr. Long's award amounts to $260,000 over 5 years, with no restrictions.

The fellowship candidates are selected from among a wide diversity of professions and are proposed by the foundation's 100 anomyous nominators. Recipients are chosen by a selection committee and the MacArthur board. Dr. Long was recognized for her work using genetic engineering techniques to improve agriculture.

Her support from the Division of Energy Biosciences focuses on the symbiotic relationships of Rhizobium bacteria and leguminous plants for possible extended uses of biological nitrogen fixation for energy conversion.

Professor Savage Inducted Posthumously as a Fellow in ASM International

The late Dr. Warren F. Savage, formerly Professor Emeritus of Welding Engineering at Rensselaer Polytechnic Institute (RPI), has been inducted posthumously as a Fellow in ASM International (previously known as the American Society for Metals). Dr. Savage was known for his many contributions to the discipline of welding science including being a codeveloper of the "Gleeble," which was a forerunner of contemporary computerized finite element programs that could simulate the complex three-dimensional and time-dependent distribution of temperature, cooling rate, and residual stress across the volume of heat-affected material that surrounds a weld interface, and of the modelling of weld behavior in terms of its dependence upon weld microstructure and welding parameters.

Dr. Savage also trained many of the leaders in welding science and engineering at RPI, with their principal funding being provided by over 12 years (1973-1986) of continuous support from the Materials Sciences program.

Young BES Grantee Honored

Professor Thomas R. Rizzo of the Chemistry Department at the University of Rochester has received support as a starting assistant professor since 1988 from the DOE for research on the chemistry of highly excited vibrational states. On the basis of his BES-supported research, he has received an Alfred P. Sloan Fellowship and has also been promoted to Associate Professor with tenure. Most recently, though, he has been notified that he is the recipient of the 1992 Coblentz Award. Sponsored by the Coblentz Society, the award recognizes significant contributions to the field of vibrational spectroscopy by a scientist under the age of 36. The Coblentz Society was formed in 1953 to foster the understanding and application of vibrational spectroscopy and now consists of over 1,000 members.

The study of chemical dissociation dynamics of molecules in highly excited states is at the frontier of chemical physics research, and has a direct bearing on combustion processes because the vibrationally excited molecules are characteristic of the high temperature environment of combustion. The studies are particularly challenging because of the complexity of the energy states which have so far eluded characterization.

Three BES Researchers Win 1991 Lawrence Award

Drs. Zachary Fisk of Los Alamos National Laboratory, Peter Schultz of Lawrence Berkeley Laboratory, and Richard Smalley of Rice University were among the six 1991 E. O. Lawrence Award recipients for outstanding contributions in the field of atomic energy. Dr. Fisk, a physicist, won in the materials research category for the discovery and synthesis of new and novel magnetic and superconducting materials; Schultz was the life sciences category winner for his contributions to the interface of life sciences and chemistry including the generation of catalytic antibodies; and Smalley received the chemistry category award for his research on the generation and characterization of atomic clusters. Dr. Fisk is supported by the Division of Materials Sciences, Dr. Schultz is supported by the Division of Materials Sciences and Energy Biosciences, and Dr. Smalley is supported by the Division of Chemical Sciences.

Energy Biosciences Grantee Elected to Academie des Sciences

Dr. Martin Gibbs, Professor of Life Sciences at Brandeis University and longtime Division of Energy Biosciences grantee, was elected as a foreign member of the Academie des Sciences of the Institut de France. Dr. Gibbs, who early in his career was a staff member at BNL and later Cornell and Brandeis, has been an active researcher on the carbon metabolism of algae and photosynthetic bacteria. He has been a member of the U.S. National Academy of Sciences for many years.

Rumford Premiums Awarded to Argonne National Laboratory (ANL) Investigators

In 1796, Benjamin Thompson, Count Rumford, presented a gift to the American Academy of Arts and Sciences for recognition of "the most important discovery in heat or in light made on any part of the continent of America or in any of the American islands." Rumford Premiums for 1992 were awarded to James R. Norris and Joseph J. Katz, of the Chemistry Division of ANL, as well as to George Feher, of the University of California, San Diego, at the annual Academy meeting recently held in Cambridge, Massachusetts. Norris is the group leader in photosynthesis research at ANL, and Katz is the former group leader, now retired. The three scientists were recognized for "outstanding contributions to understanding photosynthesis."

National Academy of Sciences Elects BES-Supported Researchers

During its 129th Annual Meeting on April 28, 1992, the National Academy of Sciences announced the election of 59 new members in recognition "of their distinguished and continuing achievements in original research." Seven of the new members receive research support from BES:

Name	Affiliation	Supporting BES Division
Jan D. Achenbach	Northwestern University	Engineering and Geosciences
George E. Bruening	University of California	Energy Biosciences
John D. Corbett	Ames Laboratory	Materials Sciences
Hans Kende	Michigan State University	Energy Biosciences
Richard R. Schrock	Massachusetts Institute of Technology	Chemical Sciences
Harry L. Swinney	University of Texas	Engineering and Geosciences
Jan Tauc	Brown University	Materials Sciences

Multiple Honors to Welding Scientist Dr. S. David of Oak Ridge National Laboratory

The Board of Directors of the American Welding Society (AWS) has designated Dr. Stanislaus A. David of the Metals and Ceramics Division at Oak Ridge National Laboratory (ORNL) as the 1993 recipient of the Comfort A. Adams Lecture Award. Dr. David will deliver that honorary lecture on April 25, 1993. This award is given by the AWS "as a means of recognizing educators whose teaching activities are considered to have advanced the knowledge of welding of the undergraduate or postgraduate students." Dr. David, and the entire welding program at ORNL, have been very interactive with both the university and industrial welding research communities. The BES welding research program is the only government program in the U.S. that supports basic research in welding science.

In a totally separate matter, the AWS has designated Dr. David for honorary membership in the Society. Their citation recognizes his "acknowledged eminence" in the welding profession, his "exceptional accomplishments in the development of the art and science of welding" and that he "has served the welding community of this nation with great distinction as an individual knowledgeable in the science and application of welding." Dr. David's other honors include being named a fellow of ASM International, a past recipient of the AWS's James F. Lincoln Gold Medal and Charles H. Jennings Memorial Awards, three Jacquet-Lucas Gold Medal awards from the International Metallographic Society and ASM International, and being designated a Corporate Fellow by Martin Marietta Energy Systems on February 26, 1992, in recognition of his "continuing accomplishments in the field of welding science and technology."

American Ceramic Society Honors New Fellows

Dr. Bruce C. Bunker (Pacific Northwest Laboratory), Professor Raj N. Singh (University of Cincinnati), and Professor Anil V. Virkar (University of Utah), all of whose research is supported by the Materials Sciences program, and Bob Gottschall of that program were honored as new Fellows of the American Ceramic Society in Minneapolis on April 14, 1992.

Combustion Scientist Honored by the Society of Automotive Engineers

Dr. Charles Westbrook of the Lawrence Livermore National Laboratory (LLNL) has received this year's Horning Memorial Board Award. The Horning Award is presented annually by the Society of Automotive Engineers (SAE International) to the authors of the best paper of the year presented at an SAE meeting and relating to the adaptation of fuels and internal combustion engines. The paper entitled, "The Autoignition Chemistry of Paraffinic Fuels and Pro-Knock and Anti-Knock Additives: A Detailed Chemical Kinetic Study," was coauthored with William Pitz also of LLNL and William Leppard of General Motors. The following paragraph is taken from the letter to Dr. Westbrook informing him of the award (emphasis added):

> "While the award recognizes specifically the contributions of [your paper] to the underlying chemical processes governing the autoignition that leads to engine knock, we recognize that this work represents the culmination of many years of work with many coauthors and colleagues. Of particular note is the correlation you have now developed between universally used research octane number and the ignition delay time predicted by your model. For the first time we now have computational tools to predict *a priori* the knock resistance of fuels and fuel blends."

Dr. Westbrook is supported, in part, by the Chemical Sciences Division of BES for the modeling of combustion chemistry.

Professor Smalley Receives Robert A. Welch Award in Chemistry

The April 13, 1992, issue of Chemical and Engineering News carried the announcement that Professor Richard E. Smalley of Rice University is the recipient of the 1992 Robert A. Welch Award in Chemistry. Professor Smalley has been supported by the Chemical Sciences Division for research on the properties of metal clusters and molecular free radicals since 1978, shortly after he joined the faculty at Rice University. Professor Smalley has attracted much attention in recent years for his codiscovery with Harry Kroto in England of the now famous fullerenes (the so-called buckyballs). This discovery and Professor Smalley's subsequent work were made using techniques and equipment developed by him with support from DOE. The Robert A. Welch Award is given annually to a chemist who has made significant chemical research contributions.

American Academy of Arts and Sciences Elects Materials Science Researchers

Three Materials Sciences researchers were elected Fellows of the American Academy of Arts and Sciences at its 212th Annual Meeting held on April 8, 1992, in Cambridge, Massachusetts. The researchers are: Francis J. DiSalvo, Jr., Department of Chemistry, (Cornell University), Royce W. Murray, Department of Chemistry, (University of North Carolina at Chapel Hill), and Douglas J. Scalapino, Department of Physics, (University of California at Santa Barbara). The Academy was founded in 1780 by John Adams "to cultivate every art and science...."

Chemical Sciences Researcher Receives Honorary Doctorate

Professor Jan V. Sengers of the University of Maryland and his wife, Dr. Anneke Sengers, a principal scientist at NIST, were recently awarded honorary doctor degrees by the University of Delft, Netherlands, on the occasion of the 150th anniversary of the university. They were both nominated by three different departments: namely, Technical Physics, Chemical Engineering, and Mechanical Engineering. It is most unusual for a husband/wife team to be so recognized. Professor Sengers has received support from the Chemical Sciences program for work on the thermodynamic properties of fluids in the near critical region. He is a recognized leader in the field of thermodynamics of fluids, and has made substantial contributions in developing cross-over theory from the region of the critical point to regular fluid behavior. Dr. Anneke Sengers has been an active collaborator with BES-supported projects and a reviewer of BES programs.

Chemical Sciences Investigator Receives Electroanalytical Chemistry Award

Dr. Stephen W. Feldberg of Brookhaven National Laboratory received the Charles N. Reilley Award from the Society for Electroanalytical Chemistry. The award was presented during a special symposium at the Pittsburgh Conference recently held in New Orleans. Feldberg is best known for his computer simulations of electrochemical and photoelectrochemical phenomena, ion and electron transport in membranes, and fast interfacial processes.

The Life Sciences Research Foundation (LSRF) post-doctoral fellowship selections for 1992 are nearing completion. Only 15 fellowships are awarded out of over 650 applications received. Three awardees are to be funded by the Energy Biosciences program. These are: Dr. Scott A. Ensign (Ph.D., University of Wisconsin) who will work on anaerobic methane and methanol oxidation in photosynthetic bacteria at Oregon State University; Dr. Cynthia A. Lincoln (Ph.D., Indiana University), who will do a molecular characterization of a developmental mutant in Arabidopsis at the USDA Plant Gene Expression Center in Albany, California; and Dr. Erica J. Pascal (Ph.D., University of California-Berkeley), who will study proteins involved in cellular transport of molecules from infected to healthy plant cells at the University of Illinois. The LSRF postdoctoral fellowships have a tenure of 3 years. Other sponsors are mostly industrial firms.

Federal Laboratory Consortium 1992 Award of Excellence for John Clarke

Dr. John Clarke from Lawrence Berkeley Laboratory has won the Federal Laboratory Consortium's 1992 Award for Excellence in Technology Transfer for the development of High-T_c superconductor device technology which is being marketed by Conductus, Inc. He is one of 30 recipients nationally. The award was presented to John Clarke on May 6 in Indianapolis. Dr. Clarke is supported by the Division of Materials Sciences.

American Physical Society (APS) High Polymer Physics Prize to Philip Pincus

The American Physical Society (APS) will award its 1992 High Polymer Physics Prize to Professor Philip Pincus, Materials Department and Chemical and Nuclear Engineering Department, University of California at Santa Barbara. The Prize was established by an endowment from the Ford Motor Company to recognize outstanding accomplishment and excellence in contributions to high polymer physics research. Pincus' work is supported by the Division of Materials Sciences. The Award Symposium will be held on March 16, 1992, during the March meeting of the APS in Indianapolis, IN. The Award citation reads: "For insightful contributions to the theory of complex polymer fluids." The APS News (March, 1992) cites, among other of Pincus' contributions, his "scientific leadership for the first synchrotron study to measure the concentration profile for polymers near interfaces...."

American Physical Society Fellowships Announced

Annually, the American Physical Society (APS) elects a small number of members to Fellowship status who have demonstrated exceptional leadership or made significant contributions to physics. This year, 172 Fellows in all fields represented by the society were so honored. Of these, 10 are principal investigators supported by the Division of Materials Sciences (DMS); 6 of 30 new Fellows from the APS Division of Condensed Matter Physics are DMS supported and 2 of 8 from the Division of Materials Physics are DMS investigators.

Professor Armstrong Receives 1992 ISCO Award for Achievements in Chemical Separations

Daniel W. Armstrong, a Professor of Chemistry at the University of Missouri-Rolla, is being honored with the 1991 Isco Award for his research in developing new chemical separations. The Isco Award was established to recognize scientists in the field of chemical separations. Armstrong is being cited "for developing a process to separate mirror-image molecules." Professor Armstrong's program, "Molecular recognition of enantiomeric Hydrocarbons by Liquid Functionalized Cyclodextrins: A New Approach for Geochemical Research" is supported by the BES-Chemical Sciences Division.

Two Engineering Research Program Principal Investigators Elected to the National Academy of Engineering

Two principal investigators supported by the Engineering Research Program have been honored by their election to the National Academy of Engineering. Professor Arthur E. Bergles (RPI) has been studying the ultimate limits of heat transfer using the evaporation of thin flowing liquid films. The region of interest includes heat fluxes of the order of tens of megawatts/m^2.

The second person honored in the recent election is Dr. J.M.H. (Anneke) Levelt Sengers (NIST). She has carried out fundamental measurements of the thermophysical properties of fluid mixtures. They include hydrocarbons, and, more recently, environmentally benign refrigerants.

Chemical Sciences Grantee is ABC World News Tonight's "Person of the Week"

A feature of the ABC World News Tonight broadcast each Friday is the naming of a "Person of the Week." On the evening of February 14, Peter Jennings gave that honor to F. Sherwood Rowland with the accolade "We have chosen a man to whom every man, woman and child owes a debt of thanks." This was the result of President Bush ordering manufacturers to end by 1995 all production of those chemicals, including chlorofluorocarbons, that are destroying the ozone layer faster than previously imagined. Jennings continues, "The person we have chosen has been warning us all about this for almost 20 years." Supportive comments came from Michael Oppenheimer (Environmental Defense Fund) and Senator Albert Gore (D-Tennessee). Jennings ended his comments with "An so we choose Sherry Rowland because he was right. The popular Science magazine once referred to him as the man who saved the planet. Maybe. Maybe now that the world is listening." Rowland's initial work on the chemistry of chlorine-containing compounds was supported by the Chemical Sciences Division.

Westinghouse Science Talent Search Finalist Supported by BES Grant

Diahung Duong, 18, of Townsend Harris High School in New York City, was named a finalist last week in the Westinghouse Science Talent Search based on his research project in polymer physics which was a part of a Materials Sciences/Office of Basic Energy Sciences supported program at Queens College of the City University of New York. Duong has received considerable press attention in New York City due to the fact that he was a "boat person," recovered off Vietnam at age 5. In the spring of last year, he received a certificate of achievement from Secretary Watkins for his entry in the Citywide Science and Engineering Fair (he was also a winner in that Fair). Duong presented the results of his research at the March 1992, meeting of the American Physical Society.

Seven Basic Energy Sciences (BES) Grantees Receive National Science Foundation (NSF) Faculty Awards for Women

Seven outstanding female science and engineering professors who receive research support from BES were selected to receive NSF's Faculty Awards for Women. This is the first time that NSF has given the awards which provide winners with up to $50,000 in research funds each year for 5 years. The awards are designed to recognize the accomplishments of women in research and teaching and to increase the number of women moving into senior ranks and positions of leadership in our Nation's colleges and universities.

One hundred awards were announced in a wide range of scientific fields including biology, behavioral and social sciences, mathematical and physical science, engineering, computer and information science, and geosciences. The awardees are:

Awardee	Institution	BES Subprogram
Sylvia T. Ceyer	Massachusetts Institute of Technology	Chemical Sciences
Lorna J. Gibson	Massachusetts Institute of Technology	Materials Sciences
Sharon R. Long	Stanford University	Energy Biosciences
Hanna Reisler	University of Southern California	Chemical Sciences
Geraldine L. Richmond	University of Oregon	Materials Sciences
Angelica M. Stacy	University of California (LBL)	Materials Sciences
Patricia A. Thiel	Iowa State University (Ames Laboratory)	Materials Sciences

Professor Macdonald Receives Two Awards for Research on Low Corrosion Alloys

Dr. Digby D. Macdonald, Professor of Materials Science and Engineering and Director of the Center for Advanced Materials, Pennsylvania State University, was awarded the 1991 Carl Wagner Award by the Electrochemical Society at its Fall meeting in Phoenix, Arizona, in October 1991. He had recently been notified of being selected to receive the 1992 Willis Rodney Whitney Award from the National Association of Corrosion Engineers (NACE). Both awards were based on the fundamental studies on passivity and passivity breakdown that Professor Macdonald has performed under a Division of Materials Sciences (DMS) grant with Stanford Research Institute and, more recently, with Pennsylvania State University. The results of this research are now having a significant impact on how alloys are designed for superior corrosion performance and, hence, for improving the energy efficiency of industrial systems. He recently presented an extrapolation from his research at the "Fifth International Symposium on Environmental Degradation of Materials in Nuclear Power Systems - Water Reactors," in Monterey, California, that "caused quite a stir because it indicates that not all is well with hydrogen water chemistry for protecting reactor internals, according to Professor Macdonald.

Professor Suresh Receives Ross Coffin Purdy Award for Ceramics Paper

Professor Subra Suresh of Brown University was named the 1992 winner of the American Ceramic Society's Ross Coffin Purdy Award. The Purdy Award is given each year for the paper judged to have made the most valuable contribution to the ceramic technical literature. Professor Suresh, along with T. Nakamura, Y. Yeshurun, K. H. Yang and J. Duffy, authored a paper entitled "Tensile Fracture Toughness of Ceramic Materials: Effects of Dynamic Loading and Elevated Temperatures." They presented new experimental methods for determining the pure tensile fracture initiation toughness in ceramics and ceramic composites and reported measurements of the dynamic fracture toughness of alumina (ceramic aluminum oxide) from 20 to 1300 °C. Knowledge of the dynamic toughness of ceramic materials is critical to their use in high-performance propulsion systems where high dynamic mechanical and thermal loads at high temperature may result in component failure with catastrophic consequences for these systems. The work of Professor Suresh and his colleagues has been at the forefront in the establishment of dynamic test methods and their interpretation for ceramic materials. His work is supported by the Division of Materials Sciences.

Joseph Darby, Jr., Honored at the Fifth International Conference on Fusion Reactor Materials

Dr. Joseph Darby, Jr., of the Division of Materials Sciences and Dr. Michael W. Guinan of Lawrence Livermore National Laboratory, who is presently serving on an assignment to the Division of Materials Sciences, both participated in the Fifth International Conference on Fusion Reactor Materials held November 17-22, 1991, in Clearwater Beach, Florida. Over 50 papers (12% of the total) presented were on fundamental studies of radiation effects in materials, which attests to the perception that radiation-induced behavior of materials may be a limiting factor in the development of fusion technology. Of these 50 papers, 40 were from abroad and 10 were from the United States.

Dr. Darby was honored by being presented a Distinguished Editor Award at the Conference Banquet. The citation read, "for his exemplary leadership of the Journal of Nuclear Materials (V50 - 1972 through V171 -

1990), for his high standards of quality and fairness, and for his contributions to the development of nuclear materials." Dr. Guinan served on the Program Committee for this conference, which was sponsored by the Office of Fusion Energy.

Dr. John D. Vander Sande Honored With the First Cecil and Ida Green Distinguished Professor Award

Materials Sciences grantee, Professor John B. Vander Sande of the Department of Materials Science and Engineering at the Massachusetts Institute of Technology, has been selected to be the first Cecil and Ida Green Distinguished Professor commencing July 1, 1991, for a 5-year renewable term. This chair is offered in recognition of his outstanding contributions to research in material science and his longstanding commitment to undergraduate and graduate education. He has pursued research on the processing-structure-electrical properties relationships in high temperature superconducting oxides under a DOE grant. His group has been using the unorthodox processing route of oxidation of metallic precursors to generate superconducting oxide/silver microcomposites. When this basic oxidation process is followed by a series of deformation and annealing steps, to induce a texture in the oxide, critical current densities in excess of 10,000 A/cm^2 at 77 K in zero field have been achieved, thereby demonstrating that this approach is a viable alternative to the oxide power-in-tube or directional solidification methods used by others. Vander Sande has strong collaborations with American Superconductor Corporation, whose President, Greg Yurek, was the previous principal investigator on this grant.

Dr. Lynn Rehn Elected Fellow of the American Physical Society

Dr. Lynn Rehn of Argonne National Laboratory has been elected to Fellowship in the American Physical Society. Dr. Rehn was cited "for significant contributions to the fundamental understanding of irradiation effects in solids." His work is supported by the Division of Materials Sciences.

Energy Biosciences Grantee Most Cited Scientist

In Science, a compilation of most cited scientists was reported deriving from data collected by the Institute for Scientific Information in Philadelphia. Leading the list was Dr. Joachim Messing of Rutgers University who has contributed greatly in the area of development of gene cloning techniques. Messing was previously located at the University of Minnesota and earlier at the University of California at Davis. The papers most cited derive from support of his work by both the Energy Biosciences program and NIH. Currently, Messing's Energy Biosciences grant covers studies on the structure of protein storage genes in maize. The citation numbers are 18,229 times for 35 papers or an average of 521 citations per paper.

Geosciences Investigator Awarded the Arthur L. Day Medal

An investigator funded by the BES-Geosciences Program has received a prestigious award from the Geological Society of America (GSA). Professor Ian S. E. Carmichael, Department of Geology and Geophysics, University of California, Berkeley, received the Arthur L. Day Medal from the GSA at its Annual Meeting in San Diego in October 1991. The award annually honors a geoscientist "for outstanding distinction in contributing to geologic knowledge through the application of physics and chemistry to the solution of geologic problems." The intention of the award is "to recognize outstanding achievement and inspire further effort, rather than reward a distinguished career." Professor Carmichael is conducting a Geosciences project entitled "Experimental Measurement of Thermal Conductivity in Silicate Liquids." Two other currently supported investigators in the Geosciences Program (G. Wasserburg and S. Epstein, both at the California Institute of Technology) have also received this award in previous years.

Recognition for Principal Investigators in Engineering Research

Professor John Ross (Stanford University) has received the prestigious Irving Langmuir Award in Chemical Physics for 1992. He is well known for his many fundamental contributions to chemical physics.

Currently, supported by the BES-Engineering Research program, he is studying far-from equilibrium energy conversion processes.

Separately, Dr. H. B. Smartt (INEL) has been invited to participate as "Distinguished Speaker" at the NSF-sponsored U.S.-Argentina Workshop on Fracture and Welding. In his lecture he will report on recent progress in sensing and control of the welding process, a part of the joint INEL-MIT project supported by the Engineering Research Program.

First Foreign Honorary Membership in the Ceramic Society of Japan to Professor J. A. Pask

Professor Emeritus Joseph A. Pask, who retired from Lawrence Berkeley Laboratory over 5 years ago, has been elected to be the first foreign honorary member of the Ceramic Society of Japan, and was installed on October 18, 1991, in Yokohama, on the occasion of their first centennial. During 1991, Professor Pask served as the President of the International Symposium on Sintering and was also elected to the National Academy of Ceramics (Italy).

Another Honor for Professor Gareth Thomas

Professor Gareth Thomas, the Scientific Director of the National Center for Electron Microscopy at the Lawrence Berkeley Laboratory, has been identified as the recipient of the 1991 Albert Sauveur Achievement Award by ASM International (formerly known as the American Society for Metals). Part of the citation for Professor Thomas reads: "...for pioneering efforts in the development and applications of electron microscopy and for fostering the universal acceptance of this technique in the evolution of modern materials science." We have previously described in these reports other honors bestowed upon Professor Thomas who has just completed a term as President of the International Federation of Societies for Electron Microscopy.

Professor Glenn T. Seaborg Receives National Medal of Science

Professor Glenn T. Seaborg received the National Medal of Science in a White House Rose Garden Ceremony in recognition of his many achievements in nuclear chemistry and his efforts to promote science education. He was 1 of 38 awardees honored with this medal and the National Medal of Technology. Upon returning to the Department of Chemistry, University of California, and the Lawrence Berkeley Laboratory in 1971 after serving 11 years as the Chairman of the Atomic Energy Commission, his further research activities were supported by the BES-Chemical Sciences Division.