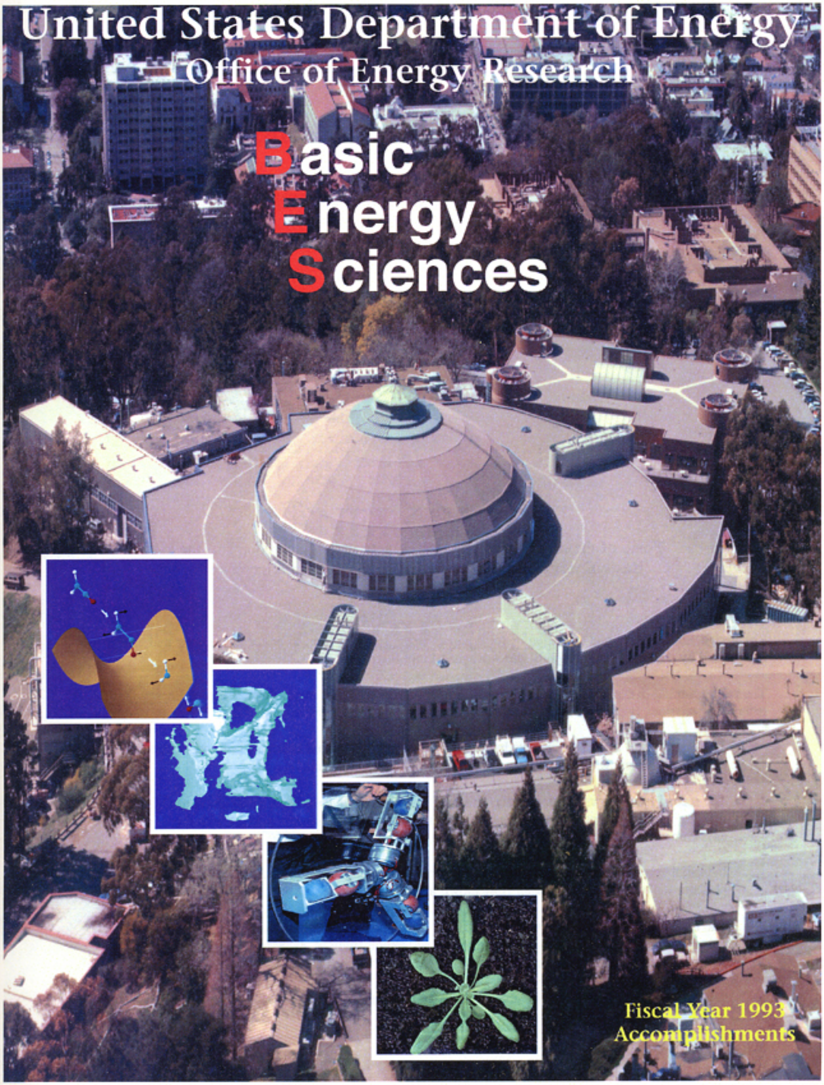
United States Department of Energy

Office of Energy Research

Basic Energy Sciences



Fiscal Year 1993 Accomplishments

Some of the many types of research activities which comprise the **Basic Energy Sciences** program are illustrated on the cover.

The design, construction, and operation of forefront scientific facilities used to understand matter and energy are represented by the aerial photograph of the Advanced Light Source (page 5).

The range of multi-disciplinary strategic research programs which impact major Department of Energy technology missions is exemplified by the four projects pictured in the overlapping insets.

The first picture, upper left, depicts basic knowledge (page 15) about chemical processes important to energy, efficiency, and environmental goals involving combustion.

The second inset shows the pore space in a sample of limestone (page 84), information useful for utilizing natural gas and oil resources or understanding how contaminants interact with the environment.

Industrial competitiveness will be enhanced by the engineering research that produced the mobile platform for robotic vehicles (page 108) shown in the third inset.

The utilization of biotechnology for the efficient production of materials, industrial feedstocks, and renewable fuels is being accelerated through the systematic study of *Arabidopsis* (page 11), the common plant pictured in the bottom inset.

Page numbers refer to marked* accomplishments.

United States Department of Energy

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BASIC

ENERGY

SCIENCES

FISCAL YEAR 1993
ACCOMPLISHMENTS

The Basic Energy Sciences staff thanks

Dr. Louis C. Ianniello

for his enthusiastic stewardship of the BES program
and wishes him well in his retirement from Federal service.

Table of Contents

This report is a compilation of some of the activities and highlights of the Office of Basic Energy Sciences (BES) during Fiscal Year 1993. It is for the internal use of the Department of Energy and other parties interested in better understanding the contributions of the BES program. This booklet is intended to spark further communication, aid in planning and analysis, and provide a source of examples of the day-to-day accomplishments of the BES program. As such a working tool, this report was not expressly prepared for public dissemination; however, its distribution is not in any way restricted.

Introduction

The Office of Basic Energy Sciences (BES) provides science and engineering research that helps enable the Department's technology development programs to succeed in their missions. By expanding the Nation's scientific and technical knowledge base and facilitating its transfer to DOE's energy technology programs and U.S. industry, the BES program invests the taxpayer's dollars to improve our country's immediate and long-term prosperity. The BES program annually funds over 1,300 research projects at about 200 U.S. universities, DOE laboratories, and industrial institutions.

A major function of the BES program is the design, construction, and operation of complex scientific facilities at the DOE national laboratories for use by the research community to conduct experiments in basic research in areas that underpin the Department's energy objectives and support the U.S. scientific enterprise. Many areas of modern science require these major facilities to develop information not otherwise attainable and, in general, only the Federal Government can provide the necessary funds. These facilities primarily include synchrotron light sources and neutron sources that are necessary to probe atomic and molecular structures and properties required to advance the fields of materials, medical, chemical, and biological science.

The BES program 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 and operating budgets are shown on page 3. The research supported by BES results in over 11,000 published reports of scientific findings in peer-reviewed journals annually.

The accomplishments for Fiscal Year 1993 provided here were regularly reported to Energy Research management throughout the year. This selection of highlights does not reflect the full range of activities under the program; however, it does provide examples of how basic research can contribute to solving a wide variety of energy-related problems and spur industrial competitiveness and economic growth.

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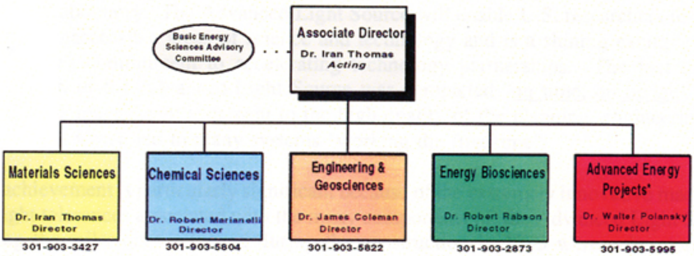
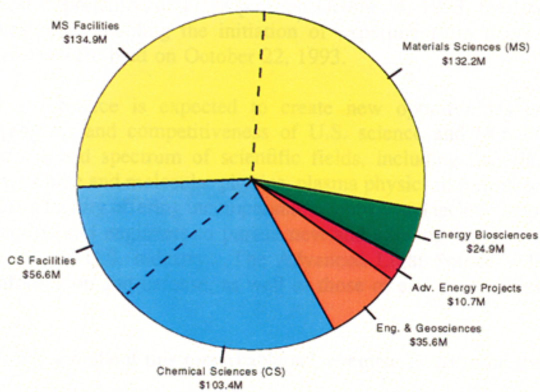
Organization and Budget

Office of Basic Energy Sciences



*The Department's Small Business Innovation Research (SBIR) Program is managed under Advanced Energy Projects.

Research Program Summary Books are published annually by each Division and are available by calling the appropriate number.



FY 1993 Budget: Operating Expenses
Research = $314.5M, Facilities = $191.5M

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Major Facilities Construction Highlights

Advanced Light Source Begins Operations

Highlighted on the cover is the newly completed Advanced Light Source at Lawrence Berkeley Laboratory. The Advanced Light Source will enable U.S. researchers to pursue otherwise inaccessible areas of science and technology and is a shining example of the Department's commitment to accelerating technology partnerships. The fact that the construction of the Advanced Light Source was completed "on time, on budget, and it works!" is a magnificent testament to the high quality of the planning, engineering, and construction which led to many systems "working the first time".

This achievement is particularly significant because of the extremely innovative machinery and tight tolerances associated with the many components of the Advanced Light Source. Among the milestones achieved during the construction in 1993 were: the storage of electrons in the ring was accomplished for the first time on March 16, 1993; on March 24, 1993, one week ahead of schedule, and the electron beam current of 65 milliamperes exceeded the 50 milliamperes baseline performance requirement for project completion; on April 9, 1993, the electron beam current reached 407 milliamperes, exceeding the goal for operation; most importantly, at 11:34 p.m. on October 4, 1993, the first light was passed down a beamline, enabling the initiation of experiments in fiscal year 1994. Dedication ceremonies were held on October 22, 1993.

The Advanced Light Source is expected to create new opportunities essential for maintaining the progress and competitiveness of U.S. science and technology. This facility will serve a broad spectrum of scientific fields, including materials research, biology, chemistry, atomic and molecular physics, plasma physics, the earth sciences, and medical science. As a facility offering incomparable scientific and technical opportunities, it will enable scientists and engineers to pursue new and exciting areas of science and technology invaluable to U.S. industry. The Advanced Light Source will affect the technologies of information and defense, as well as those of energy, transportation, and health.

More detailed information about this remarkable achievement is given on the following two pages.

Background Information on the Advanced Light Source

The National Laboratories were erected in the 1940s and 1950s to foster scientific and engineering education and research to improve the quality of life for Americans. To maintain scientific and technical leadership, more and more highly sophisticated facilities such as synchrotron light sources are required to probe the atomic and molecular structures for materials, chemical, biological, pharmacological, and medical research. The understanding of the behavior and properties of materials undergirds every major technology area, including those of information and communication systems, computers, energy production and use, health, transportation, and national security. It could be said that every technology is "materials-limited."

These important research facilities are built and operated at DOE's laboratories with BES support. The collocation of advanced high-technology research equipment, leading-edge expertise of staff scientists and engineers, and visiting users from a wide variety of scientific disciplines provides the Nation with an invaluable asset. State-of-the-art facilities, such as the Advanced Light Source, are available to industrial, academic, and government researchers in the realization that America's position in world science and in the global economy can best be advanced through close association between strategic basic research and technology development, and between the public and private sectors.

The Advanced Light Source produces electromagnetic radiation (light) by confining electrons to orbits within a storage ring. When the electrons' paths are bent by magnets, they emit light tangential to the electronic orbit. The light, called synchrotron radiation, is a natural consequence due to the acceleration of the electrons. Depending on the energy of the electrons, the energy type of the light emitted by the machine can vary.

Sophisticated instruments are attached to the outside of the storage ring to utilize the light for determining the structure and properties of matter. Many such instruments, used in different experiments, are attached around the storage ring, forming many beam lines. The brighter the light, the more information scientists can gain from their samples per unit time.

The sciences which focus on condensed matter, or materials research in general, deal with the properties of solids and liquids and their interfaces. They are inter-disciplinary, involving materials sciences, major areas of physics and chemistry, the earth sciences, biology, and medicine. The understanding of the behavior and properties of materials is essential to national capacities in advanced technology and, hence, to economic competitiveness.

Condensed-matter science supports advanced technologies in areas of national priority, including those of information systems, communication and computers, energy, health, transportation, and national security. Products of condensed-matter science such as the transistor, the integrated circuit chip and liquid crystal displays, have revolutionized our lives through their use in television, calculators, electronic watches, personal computers, appliances, autos, and innumerable other applications.

All science depends on advanced instrumentation to enable scientists to see phenomena they have not observed before. Synchrotron radiation provides the most intense source of light now available over a broad spectral range. Such radiation can be intensified further by orders of magnitude by using insertion devices--wigglers and undulators--that put a series of bends in the electron trajectories. Synchrotron-produced photons interact strongly with atomic electrons, thus, making it possible to probe the details of the electronic structure of materials.

Research with synchrotron radiation began in the 1960s and has grown dramatically. Each decade has seen the development of a new generation of synchrotron light sources offering orders of magnitude increases in brightness, enabling new types of research to become possible. Furthermore, experiments carried out with such new equipment have demonstrated how new science could be developed if still higher brightness was available.

With the completion of the Advanced Light Source, we have gone through three generations of such increases in brightness. The first was associated with synchrotron radiation from the bending magnets of storage rings built for particle or nuclear physics. The second came with the construction of new storage rings specifically intended to produce synchrotron radiation. The third generation of synchrotron radiation facilities, realized in machines such as the Advanced Light Source, involved the construction of storage rings designed to maximize the brightness of the radiation from insertion devices. Such facilities offer brightness increases by factors of from 50 to more than 100 over past synchrotron radiation facilities.

The Advanced Light Source is centered around insertion devices optimized for high brightness in the soft x-ray and extreme ultraviolet synchrotron radiation regions. The growth of research using these spectral regions has paralleled that in the x-ray region, hence, the Advanced Light Source provides the Nation with a truly complementary resource to the Advanced Photon Source now under construction at Argonne National Laboratory, which will provide hard (more energetic) x-ray beams. The brightness of the light depends on the magnitude of the current and the energy of the electrons in the storage ring (measured in milliamperes).

Ultraviolet radiation is in the energy range from 10 to about 100 electron-volts. It is useful for studies of the electronic properties of microstructures, surfaces, ultra-thin layers, and small clusters. Soft x-rays have energies ranging from about 100 to about 2,000 electron-volts. They are used in a wide range of electronic structural studies and are particularly useful for x-ray lithography. The Advanced Light Source, therefore, is the optimum storage ring energy for producing undulator radiation with wavelengths in the range of 10 Angstroms and greater, offering special opportunities for research in chemical physics, electron spectroscopy, microscopy, and holography.

Advanced Photon Source Proceeding on Schedule

Beneficial Occupancy of the Early Assembly Area

On December 23, 1992, the Advanced Photon Source (APS) project was granted Beneficial Occupancy of the Early Assembly Area by the Department of Energy's Argonne Area Office. This occupancy is a pivotal event in the ongoing process of designing, fabricating, and installing the accelerator systems. It provides working space for the testing of accelerator magnets, and the assembly of magnets and vacuum chambers on girders prior to their installation in the storage ring. These activities are vital tasks on the critical path that leads to completion of the accelerator storage ring. Once the storage ring installation activities are complete, the Early Assembly Area will house offices, assembly space, and large laboratories for several technical groups.

The area will house a magnetic-field mapping facility, a girder staging and assembly area, a machine shop, a 15-ton crane, two mezzanines for heating, ventilation and air conditioning and electrical equipment, and sanitary facilities. The Advanced Photon Source Project is supported through the Office of Basic Energy Sciences/Materials Sciences Division.

Title II Design Approved for the Insertion Device Magnetic Measurement Facility

On November 30, 1992, the APS completed a milestone set by the Project Manager of the Department of Energy Argonne Area Office. An external review team chaired by Dr. Mike Green of the Synchrotron Radiation Center, Stoughton, Wisconsin, approved the Title II Design of the Insertion Device Magnetic Measurement Facility. This facility will be used for magnetic-field mapping of all insertion devices (IDs) used for the production of the brilliant X-ray beams at the APS. Field mapping provides information on such critical qualities as beam stability and spectral performance of the IDs.

The Insertion Device Magnetic Measurement Facility will consist of a 6-m-long precision granite bench equipped with a set of different magnetic probes, a system of electronics, and mechanical systems capable of driving the magnetic probes in three directions with the very high accuracy (1-10 microns) required for magnetic field mapping of 5-m-long IDs. The software required to run the electronics and analyze the data from the measurements has already been developed to operate the engineering model. The facility will be capable of performing automated, unattended tasks for days while acquiring thousands of measurements.

In their final report, the Title II Design Review Committee stated that "the Advanced Photon Source is to be complemented for anticipating the importance of a level of effort necessary in making magnetic field measurements of insertion devices for the third generation synchrotron radiation sources...Based on the material presented and the competence of the APS staff, the Committee is highly confident of the successful operation of the proposed expansion of the Magnetic Measurement Facility."

Exemplary Safety Continues

The Advanced Photon Source at Argonne National Laboratory continues to meet its cost and schedule goals and to set an impressive safety record. While U.S. building construction has an average of 6.5 accidents per 200,000 hours and the Department of Energy construction has an average of 2.7 accidents per 200,000 hours worked, the Advanced Photon Source has only 1.2 accidents per 200,000 hours worked with over 55 percent of the work completed. In research and development, the safety at the Advanced Photon Source is as impressive. The U.S. average is 1.4 accidents per 200,000 hours and the Department of Energy average is 1.1 per 200,000 hours. At the Advanced Photon Source the accident rate for research and development is 0.4 accidents per 200,000 hours.

Dr. Richard Hislop of the Advanced Photon Source has been awarded (October 1992) the Robert M. Farrell Memorial Safety Award for 1992 by the Construction Safety Association of America, Inc. (CSAA) in recognition of his efforts toward promoting construction-safety awareness. Construction contractors working on the APS, and those construction contractors working at ANL after 1991, were required by ANL to compile documented safety programs. Those contractors subsequently made use of these safety programs when performing work in the greater Chicago area. The APS Project safety requirements, which have been formally adopted by ANL, have resulted in a greater awareness of safety within the Chicago-area construction community at a time when a new initiative was needed to encourage further improvements in construction safety.

The CSAA had its genesis in the first Chicago-area Occupational Safety and Health Administration training course, held in February 1971. Following that meeting, it was decided to establish the CSAA as a way to keep members of the Chicago construction community abreast of developments relating to the Occupational Safety Administration Act.

In 1978, the CSAA established an annual award recognizing outstanding contributions to construction safety in the Chicago area. This award was named in honor of Robert M. Farrell, who was the safety director for Local 150 International Union of Operating Engineers (Ohio to southern Illinois) and president of the CSAA. Farrell made major contributions to the development of the CSAA, and to the promotion of safety throughout the Chicago-area construction industry.

<u>User Housing Facility to be Built by Illinois</u>

The Advanced Photon Source is a national user facility being built at the Argonne National Laboratory with funding from the Department of Energy. When the facility operates in 1996, about 500 scientists, engineers, and graduate and undergraduate students from universities, industries, and national laboratories will be using the facility.

The State of Illinois made a commitment to build User Housing when the project was proposed in 1986 to provide the Advanced Photon Source user with accommodations on the Argonne National Laboratory site. In keeping with this promise, the State of Illinois, in its appropriations passed on July 13, 1993, has set aside $1.5 million for fiscal year 1994 (starting July 1, 1993) to begin the design work and preliminary site preparation. The balance of funding needed to complete the facility (currently estimated at $17.3 million) is expected to be appropriated by the State of Illinois in fiscal year 1995 and fiscal year 1996. The building, with over 125,000 square feet, will accommodate about 240 beds for the Advanced Photon Source users and will contain modest kitchen, dining, laundry and meeting facilities. The current plan calls for its completion in 1996.

Secretary O'Leary wrote the Governor of Illinois on May 28, 1993, urging the State of Illinois to follow through on its promise to build the facility.

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Basic Scientific Advances

Examples of Research Highlights

The Basic Energy Sciences program supports strategic basic research that creates new knowledge to better utilize technologies which develop energy resources in a safe and environmentally sensible manner. Hence, the program takes a broad, multi-disciplinary approach which has benefitted industries directly related to major energy systems, and also many other advanced technologies important to the social and economic well-being of the United States. This section contains brief summaries of the kinds of strategic research results which help spur future technology development and economic growth, and the types of workshops and activities that make it happen.

Gene Studies of Plants Reap Diverse Benefits*

Plants, like other higher organisms, undergo complex developmental changes during their life cycle and, therefore, offer many opportunities to scientifically explore the biological mechanisms involved in gene regulation during their development. A common plant, *Arabidopsis thaliana* (shown in the fourth inset (lower right) on the cover of this booklet*), is used extensively in such molecular studies, since the plant is very small (about the size of a fifty cent coin), grows quickly (from seed to seed in six weeks), and possesses a relatively small genome (about one-thirtieth the size of the human genome) which facilitates many biological manipulations. For example, the September 24, 1993, issue of Science magazine features work supported by the Division of Energy Biosciences on its cover. The related research paper by Dr. Elliot Meyerowitz of the California Institute of Technology describes the activation of genes during the development of flowers in *Arabidopsis thaliana.*

Another aspect of Dr Meyerowitz's work has led to the isolation of the gene encoding the protein that is the receptor for the plant hormone, ethylene. This is the first isolation of a plant hormone receptor gene. The role of ethylene in many plant developmental processes makes this a particularly attractive target for biotechnological manipulation. It is likely that one of the first applications will be to alter the ripening of fruit (an ethylene controlled event) providing an extended shelf life for perishable agricultural products. An example of the benefits to U.S. consumers would be the ability to produce commercial tomatoes with the taste and texture associated with those "homegrown."

Yeast "Factory" Trained to Produce Plant Enzyme

A Center for Advanced Materials research team at Lawrence Berkeley Laboratory under the direction of Jack Kirsch and jointly supported by the Office of Basic Energy Sciences/Materials Sciences and Energy Biosciences Divisions has succeeded in turning yeast cells into "factories" for the inexpensive production ("expression") of the plant enzyme papain, an important target for novel polymer synthesis studies.

The gene for this enzyme was taken from its natural papaya host and inserted into yeast cells. It was then used to guide the protein synthesis in collaborative work with Dr. Shane Weber of Eastman Kodak in Rochester, New York. The key to the expression of significant quantities of enzyme, estimated to be about 8 mg/l of yeast growth media, lies in Weber's construction of an efficient, generalized yeast expression system using what he calls a "flag epitope." In this technique, genetic material coding for a protein segment known to be bound by an antibody is attached to the deoxyribonucleic acid coding for the protein of interest. The antibody can then be used to bind and "fish" out its protein segment and, along with it, the target protein.

The importance of this result lies in the role that papain can play in polymeric materials synthesis. Papain acts on its substrates through a thio-ester, rather than a oxy-ester intermediate. Thio-ester intermediates lend themselves far more readily to polymerization than do oxy-ester intermediates. The search for thio proteases led to plants (there are few, if any, in microorganisms) and thus the difficult task of expressing a plant enzyme in a microorganism such as yeast.

A central objective of the research into enzyme-mediated new materials synthesis is the redesign of proteolytic enzymes such as papain, so that instead of catalyzing the degration of natural protein polymers, they synthesize unnatural sequences of interest. This requires that they be engineered and, thus, their catalytic sites must be redesigned to recognize peptide structures that are different from those normally recognized. Cloning and expression are necessary to this redesign. While papain has been expressed in a insect-based expression system by earlier workers, the yields there are low and the process is expensive. Thus the ability to design a yeast expression system is of great value.

The economical production of peptides synthesized with this technique could make it possible to use them to produce a variety of specialized fibers.

A New Method is Developed for Better Understanding Surface Films

A new method for studying surface films has been developed with support from the Office of Basic Energy Sciences/Chemical Sciences Division by Dr. Charles B. Harris and coworkers at the Lawrence Berkeley Laboratory and the Chemistry Department of the University of California at Berkeley. The characterization of thin surface films is important in applications ranging from electronics to lubrication and environmental processes. The method, known as two-photon photoemission, is general and very sensitive to the structure and molecular composition at the interface.

The method measures changes in the image-potential states at a metal surface in the presence of thin layers of absorbed materials. The image potential is an attractive force experienced by an electron due to the surface charge redistribution induced by the electron charge. The presence of an intervening layer alters the potential and therefore the interaction of the electron with the surface. The nature of this interaction is probed using two-photon photoemission spectroscopy. The first photon promotes an electron from an occupied state in the surface to an excited state characterized by the image-potential. The second photon causes the electron to be emitted from the surface. The kinetic energy of the emitted electron is determined from the time between the second light pulse and the arrival of the electron at a detector. The angular dependence of the energy of the electron leaving the surface also contributes to the characterization of the interaction between the film and the surface.

The technique has already demonstrated greater energy resolution than obtained using other methods. Spectra from hydrocarbon layers show a rich structure with layer-by-layer shifts in binding energy. The success to date of this new approach suggests its application to a range of problems such as the localization of excess electrons in insulators, metal-nonmetal transitions, magnetic films, and the behavior of electrons at Schottky barriers. High speed detection may also reveal details about the dynamics of electrons at interfaces and in thin films.

New High Temperature Superconductors Discovered

A new high temperature superconductor, with a critical temperature at 94 Kelvins, composed of mercury, barium, and copper oxide has been synthesized and characterized using neutron powder diffraction. In research supported by the Office of Basic Energy Sciences/Materials Sciences Division, scientists at Argonne National Laboratory, and

Northern Illinois University have shown that the defect concentration of excess oxygen can be varied by annealing in different oxygen partial pressures resulting in a corresponding variation of critical temperature over the range of 44 Kelvins to 95 Kelvins. A second structural defect involving the substitution of copper on about 8 percent of the mercury crystallographic sites is probably required to stabilize the crystal structure. The compound has a single layer copper oxide superconductor. Subsequent reports have appeared concerning materials with a double or triple layer of copper oxide with critical temperatures as high as 133 Kelvins which is a new record at this point.

The new compound first reported by S. N. Putilin, et. al., in *Nature*, March 18, 1993, is of particular interest because it displays a remarkably high critical temperature for a material with a very simple crystal structure. That structure contains a single copper oxide layer and is considerably less complicated than the majority of the high temperature superconductors now known, and is particularly easy to synthesize and to incorporate a small amount of excess oxygen in the form of an interstitial defect. Ott et. al. [Nature 363, 56 (1993)] have identified a new composition which has three copper oxide layers per unit cell and believe it to be responsible for the record-setting critical temperature although this has not yet been established beyond doubt. Careful structural analysis by the Argonne scientists should establish the nature of these new materials.

Structure of Glasses Important for Nuclear Waste Storage Applications

Silicate and germinate glasses have important applications including nuclear waste storage. Central to many of these applications, as well as being an important issue in materials science, is the atomic structure of the glasses. The arrangement of the atoms in glasses differ from that in crystalline materials in that they are not arranged in a long-range periodic order, which significantly affects the properties of the material. However, it is known that the structure of glasses possesses a substantial degree of long-range regularity associated with the packing of small structural units. This regularity, known as "intermediate-range order," can be observed in diffraction patterns taken by neutrons or X-rays and also in optical spectra of glasses.

Experiments by Argonne scientists on silicate and germinate glasses have revealed an even longer range regularity, termed "extended-range order," that appears in the diffraction patterns at low angles. The origin of this new type of regularity has been explored with a combination of neutron diffraction at the Intense Pulsed Neutron Source at Argonne and "anomalous" X-ray diffraction at the National Synchrotron Light Source at Brookhaven. It is important to use both neutrons and X-rays since the structure of these glasses have three different types of atoms which have to be described in terms of the six different kinds of atom pairs, and cannot be unraveled by a single diffraction measurement. For these studies, a series of rubidium germinate glasses was chosen since the materials were ideally suited for neutron and anomalous X-ray diffraction experiments. By analyzing the data, it was possible to establish that the extended-range order is associated with chemical ordering of the rubidium and germanium atoms. This kind of ordering is well known in molten salts like sodium chloride, where the sodium and chlorine ions form an ordered arrangement. In this glass the chemical ordering is between the two types of metal atoms, accompanied by a spatial ordering of the oxygen atoms, which accommodate themselves to the metal atom structure.

This extended-range order is not found in other complex glasses, such as lead germinate, which have lower ionic conductivities, i.e., ionic mobility. A possible relation between structural regularity and ionic mobility is being explored in ongoing research. Since material stability is of crucial importance in nuclear waste storage, ionic motion of diffusion is a key property to understand.

This work represented a collaboration between Argonne (J. G. Ellison, D. L. Price, and M. Saboungi), the University of Pennsylvania (R. Hu and T. Egami), and the Rutherford Appleton Laboratory, United Kingdom (W. S. Howells). The Argonne research and the operation of the Intense Pulsed Neutron Source and the National Synchrotron Light Source are supported by the Office of Basic Energy Sciences, Division of Materials Sciences.

Novel Type of Rubbery Solid Electrolyte Discovered

Basic research on ionic transport properties in materials at Arizona State University under the direction of Professor C. Austen Angell has led to the development of a novel type of solid electrolyte with rubbery properties and high ionic conductivity. This rubbery electrolyte is a "polymer-in-salt" (low polymer, high salt content) type of material that combines the best features of superionic glasses, molten salts, and traditional polymer ("salt-in-polymer") electrolytes, while preserving a high electrochemical stability.

Although research on this new type of flexible electrolyte is only in its early stages, initial measurements on several compositions have demonstrated lithium ion conductivities as high as some of the best lithium ion solid electrolytes currently available. These results suggest that this novel type of electrolyte could be a significant breakthrough in the development of lightweight batteries for transportation, which demand high ionic conductivity and mechanical flexibility. A patent application for this novel type of electrolyte has been filed and research is now focussing on the development of new ionic polymers and lithium salts for use in preparing more advanced rubbery electrolytes.

This scientific breakthrough was reported in *Nature* on March 11, 1993, and has since been highlighted by scientific editorial reviews as well as by international press reports. A strong indication of its technological potential is the number of inquires Professor Angell has received from Japanese and German industries who have expressed interest and have indicated plans to redirect work into this area. This research was carried out at Arizona State University by C. A. Angell, C. Liu, and E. Sanchez under a grant from the Office of Basic Energy Sciences/Division of Materials Sciences.

Optical Technique Developed as Monitor for Chemical Vapor Deposition

Growth rates of materials deposited by chemical vapor deposition have been measured in real time using in situ reflectance measurements. Improved sensitivity to the growth and composition of ultra-thin semiconductor layers of silicon, silicon dioxide, gallium arsenide, and aluminum gallium arsenide has been demonstrated with this nonperturbing, easily-implemented, diagnostic. The technique has been used to examine the correlation of gas-phase diffusivities to deposition rates in metal-organic chemical vapor deposition. Measurements were made in a rotating disk metal-organic chemical vapor deposition reactor to compare the growth rate of aluminum arsenide with hydrogen versus nitrogen carrier gases. Based on fluid flow models, results indicate that growth rates scale as diffusion limited rates. Experiments are also underway investigating the potential for this in situ diagnostic as a process control sensor for monitoring the growth of precision multilayer structures typical of optoelectronic devices.

Chemical vapor deposition processes are finding broad application in advanced technology, however their effective utilization has been hampered by the lack of in situ diagnostics that can measure such fundamental parameters as growth rate and composition of the materials that are being deposited. This deficiency limits both the fundamental understanding of the mechanisms of chemical vapor deposition and the production efficiency of chemical vapor deposition manufacturing processes. This new in situ reflectance technique allows measurement of the deposition rates of chemical vapor deposition films under actual growth conditions (i.e., at high temperatures and pressures and in the presence of reactive gases). Such measurements are critical both for creating and validating physically and chemically based models of complex chemical vapor deposition processes. The method also has the exciting potential for application as a real-time process control sensor, providing critical input on layer thickness and film composition to process controllers for intelligent feedback and rapid correction of process conditions. This research continues to be supported by the Office of Basic Energy Sciences/Division of Materials Sciences at Sandia National Laboratories in Albuquerque.

Measurement of Transition State Now Possible*

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 *Science* 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. A pictoral representative of this process is shown in the first inset (upper left) on the cover of this booklet.*

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 1920s 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 are now 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.

Organometallic Models for Petroleum Desulfurization

Despite the great importance of the catalytic hydrotreating process which treats more than 27 million barrels/day of petroleum feedstocks with hydrogen over molybdenum catalysts to remove sulfur contaminants, the molecular details of the process are not understood.

Now, in a research program aimed at understanding the hydrodesulfurization process, Office of Basic Energy Sciences/Chemical Sciences Division-supported researcher, R. J. Angelici of the Ames Laboratory, finds that a combination of iron and iridium organometallic compounds provide a model for details of the molecular reactions that occur on the surface of the catalyst. How thiophene bonds to the metals and is broken apart and the sulfur removed, has been plausibly shown in sequence, with the first two steps being favored by metal catalysts in low oxidation states. Other studies by his colleague (G. L. Schrader) at Ames have confirmed that commercial-type molybdenum catalysts with the metal in low oxidation states are especially effective for thiophene hydrodesulfurization.

This detailed understanding of the hydrodesulfurization process at the molecular level could help point to ways to produce better petroleum desulfurization catalysts. Since thiophenes are among the most difficult sulfur-containing molecules to remove from petroleum fractions, and new environmental standards require severe reduction in sulfur emission levels, there is a high degree of interest in these catalytic studies which may help in the quest to produce gasoline and heating oils with very low sulfur contents.

Positron Ionization Processes Explored for Mass Spectrometry

Research done by L. D. Hulett and J. Xu of Oak Ridge National Laboratory on the ionization processes under positron (electron anti-particle) bombardment has led to the discovery of two possible ionization pathways for aliphatic hydrocarbon organic molecules. In the first ionization process, a positron having a kinetic energy greater than 3.0 eV interacts with a molecule and extracts an electron, forming the positronium atom and leaving the intact molecule ionized with a single positive charge. This positronium atom has enough kinetic energy to leave the molecule and drift away from it, undergoing positron-electron annihilation (141 nanoseconds later) at some point far removed from the molecule. In the second process, the organic molecule is bombarded with positrons having a kinetic energy less than 0.5 eV. The positron does not have enough energy to extract an electron, therefore it can annihilate with a bound electron on the organic molecule. The annihilation energy is channeled into the molecule leaving it in a highly excited state which causes the molecule to fragment into many ions. This low energy process is in direct contrast with the ionization and fragmentation processes which occur under electron bombardment, where the electron energy must be greater than the ionization threshold limit of 9-10 eV to have any effect. These new mechanisms can lead to a more fundamental understanding of ion physics and will impact gas phase ionization processes in mass spectrometry important to the difficult problems of measuring organic materials in environmental waste and industrial processes.

New Synthesis Gas Production Reported

Both the Wall Street Journal and the Washington Post reported potential new advances in the conversion of methane, the principal component in natural gas, to a transportable liquid. The new reports are based on two articles in the January 15, 1993, issue of *Science* Magazine which emphasizes two specific approaches; namely, direct conversion to methanol and the conversion to synthesis gas (CO and H_2) followed by Fisher-Tropsch processing to liquid hydrocarbons. Research on the synthesis gas conversion is supported by the BES/Chemical Science Division.

The primary problem associated with effective utilization of natural gas is economical transportation from distant sites, especially intercontinental. Methane-derived liquids are more manageable and safer than gaseous methane. The advance in synthesis gas conversion is achieved by altering the selectivity of the catalytic partial oxidation reaction and represents a marked improvement over current technology.

This advance minimizes the combustion of the methane to CO_2 and water. Professor L.D. Schmidt found the combination of catalyst and conditions while studying the free radical chemistry of surface initiated radical reactions and transport of radicals to and from the gas phase.

"Infringing on Nature's Patents"

The above quotation is the headline of a news column in the December 7, 1992, issue of the Boston Globe. The column described research results presented at the Materials Research Society's annual meeting in Boston in early December. The research involves the use or the mimicking of biological processes to make new materials. The news report featured the work of Dr. Hagan Bayley of the Worcester Foundation for Experimental Biology in Shrewsbury, Massachusetts. Dr. Bayley's work involves the construction of novel material with a selection of microscopic pores using genetic manipulation of a bacterial channel protein which is secreted by *Staphylococcus aureus*. The ability to construct pores with different internal diameters and biological uniformity will allow selectivity for the passage of molecules and ions, possibly with gated properties (the ability to open or close in response to a physical stimulus, e.g., an electric field or light). Ultimately, the new pores could be used to confer novel permeability properties to materials such as thin films. Such products have potential technological applications, for example, as components of energy conversion and storage devices, selective electrodes, electronic devices, and ultrafilters. This research is supported jointly by the BES/Divisions of Materials Sciences and Energy Biosciences.

Argonne National Laboratory Scientists have Established a World's Record for "Giant Magnetoresistance"

Argonne National Laboratory scientists have established a world's record for "giant magnetoresistance," an effect that could speed up computers and make industrial robots more precise. The material under study is a "superlattice" of iron and chromium, according to Argonne Scientist Samuel Bader who is supported by the Office of Basic Energy Sciences/Division of Materials Sciences. The superlattice consists of alternating layers of each material one million times thinner than a sheet of paper.

When a magnetic field is applied to a superlattice cooled with liquid helium, its electrical resistance decreases so that about two and a half times more electric current will flow through the material than in the absence of the magnetic field. The previous record-holder allowed a factor of two increase in electric current with the application of a magnetic field. Typical magnetoresistive materials have previously shown a resistance change of only one to two percent.

The experimental results provide a particularly stringent test of recent theoretical models which depend sensitively on orientation. For applications, this achievement is significant because of the size of the effect, which implies increased sensitivity for devices, and because sputtering is a preferred deposition technique to molecular beam epitaxy in industrial settings. Epitaxial growth via sputtering allows the magnetic properties to be tailored conveniently by controlling both the crystal orientation and the anisotropies of the magnetic layers.

Potential applications for magnetoresistive materials include ultra-sensitive "read heads" for retrieving information stored on computer disks. Read heads send pulses of electricity to the computer as they react to tiny magnetized areas - the recorded data - on a spinning disk.

The superlattice developed at Argonne is about 75 times more sensitive to magnetic fields than the nickel-iron alloys now used for magnetic heads which sense the magnetized bits of information from recorded media. It could get a better signal from a disk in a shorter time, allowing the disk to spin faster. Faster rotation decreases "access time" and allows the disk-reading process to keep pace with today's faster processors.

The superlattice also could be used in robotics and industrial automation. Position sensors made of magnetoresistive materials can provide accurate and rapid signals when an assembly-line tool reaches a designated position.

The "magnetron sputtering" process used to create the superlattice is already being used by industry to create thin films of material. Previous methods of creating giant magnetoresistive materials were complex and inefficient. Further research will focus on producing materials that show the same giant magnetoresistive effect in a lower magnetic field.

New NMR Spectroscopy Helps Characterize Yttrium Materials

Among the wide range of non-hydrated yttrium compounds are the very interesting compounds related to high temperature superconductors, e.g. $YBa_2Cu_3O_{7-x}$, and characterization of the environments about the metals are continually being sought.

Professor Evans and his group at the University of California, Irvine, have demonstrated that ^{89}Y solid state nuclear magnetic resonance spectra, using cross polarization with magic angle spinning (CP/MAS), can be easily obtained on a broad range of compounds in a short period of time. X-ray crystallography characterizations of the compounds have shown a direct correlation between the number of NMR signals and the number of unique solid state environments, and routine yttrium NMR spectroscopy on hydrate-free systems can now be an invaluable tool for studying these important systems. Impurities in yttrium-containing materials have also been quite difficult to identify and characterize, and the technique provides an easy method for rapid determination of purity in bulk samples which are not tractable by other standard methods.

Although solid state NMR spectroscopy using CP/MAS can provide useful information on solids containing nuclei such as ^{13}C, ^{27}Al, ^{29}Si, and ^{31}P, the technique does not work for low γ nuclei such as those possessing frequencies lower than ^{15}N (20.26 MHz at 4.7 T). Thus important atoms such as ^{89}Y, which resonates at 9.8 MHz were traditionally characterized by single pulse experiments with the attendant drawbacks of long relaxation times, rolling baselines, and low sensitivities. The solid state ^{89}Y resonances found by these researchers are without the aforementioned problems, span a broad range, and provide "fingerprints" characteristic of the environment around the metal.

Solvent Cage Effect Directly Observed

The 'cage effect' is one of the most important solvent effects on a chemical reaction. In an international collaboration with Israeli workers, Curt Wittig from the University of Southern California, with support from the Office of Basic Energy Sciences/Chemical Sciences Division, has obtained direct evidence of the cage effect from the photolysis of an Ar-HBr cluster. The effect manifests itself as a tail toward lower energies in the H atom photofragment kinetic energy distribution. The light H atom, initially trapped between the heavy Ar and Br atoms of the cage, collides several times before leaving the cluster. Energy transfer occurs from the light to the heavy particles resulting in the low energy tails.

The cage effect has been invoked in dissociation processes for more than 50 years. When, for example, an isolated diatomic molecule is electronically excited from its ground state to a repulsive one, the dissociation of the diatomic bond is direct and rapid, with a yield of unity. The behavior of the diatomic molecule can differ greatly from this picture when it is no longer free, but weakly bound to some solvent atoms or molecules, as in a liquid or cluster. The surrounding solvent may act as a "cage" confining the photofragments, and therefore prevent or delay their mutual separation. The results provide evidence for the large influence of even a single solvent atom on the dissociation process.

Scientists Make First Measurement on an Elusive Process

Scientists at Lawrence Berkeley Laboratory supported by the Office of Basic Energy Sciences/Division of Chemical Sciences have reported the first observation and measurement of electron capture from pair production i.e., simultaneous formation of an electron and a positron. Using a spectrometer of novel design the scientists collided a uranium ion beam extracted from the Bevalac with foil metal targets. At the high energies used for the experiment, the interaction of the ion, in close proximity to a nucleus of a foil atom, created a sufficiently strong field to effect pair production. The ion then captured the electron and was detected as an ion with a charge reduced by one.

The results were chosen by the International Conference on the Physics of Electronic and Atomic Collisions, held the summer of 1993 in Denmark, for presentation as a "Hot Topic" and is but one of ten papers so selected. The International Conference on the Physics of Electronic and Atomic Collisions was attended by over 1,000 scientists from 41 countries.

The measurement is of particular importance to design of new generation heavy ion accelerators, such as the Relativistic Heavy Ion Collider since the process may reduce the integrity of the ion beam. The experiment is one of the last experiments to be done on the Bevalac which is being decommissioned. A patent disclosure of the spectrometer has been made.

New, Efficient, Fast Scintillators for Radiation Detection

The overall performance of gamma radiation detection systems, including systems for the monitoring and control of repositories for fissile material removed from deactivated nuclear weapons, can be significantly enhanced by the development of more efficient scintillator materials with increased durability in hostile environments.

A recent Office of Basic Energy Sciences/Division of Materials Sciences-supported collaborative effort involving Oak Ridge National Laboratory and Boston University has led to the discovery of a promising new scintillator with the potential for deployment under deleterious environmental conditions and for a broad range of radiation detection and monitoring applications.

The new scintillator, cerium-doped lutetium orthophosphate has a relative light output that is over twice that of bismuth germanium oxide - a scintillator currently in widespread use. In addition the new scintillators have a response time that is twelve times faster. The new scintillator is unaffected by water vapor in the atmosphere and is not affected by most common acids in concentrated form (e.g., nitric acid, hydrochloric acid, etc.). The material can withstand temperatures up to 2000°C and is resistant to "browning" or color center formation due to high radiation doses. This latter characteristic combined with the thermal and chemical stability of the material offers the potential for the development of improved detectors for medical applications, such as positron emission tomography and for other applications requiring the deployment of radiation detectors in demanding and hostile environments. This research was carried out by Dr. L. A. Boatner of Oak Ridge National Laboratory and Professor A. Lempicki of Boston University.

Ultrasensitive Analytical Tool Characterizes Microscopic Inclusions in Minerals

J. K. Bohlke and J. J. Irvin, working under the Office of Basic Energy Sciences/Geosciences Program support at Argonne National Laboratory and the University of California at Berkeley, respectively, developed a technique capable of chemical analysis on a suite of rare gas and halogen isotopes using as little as 10 femtoliters (0.01 mm^3) of fluid contained as microinclusions in minerals. The extreme sensitivity and high spatial resolution demonstrated with this technique may offer promise in materials synthesis and characterization of ceramics. This new, ultrasensitive technique greatly extends the range of application in studies of mineral-fluid interactions.

Analyses of microscopic fluid inclusions from the hydrothermal lead-fluorite-barite deposits at Hansonburg, NM, which were deposited 30-65 million years ago, indicate an originally meteoric fluid that (1) acquired chlorine and sulfate from marine evaporites, (2) acquired ^{40}Ar and Pb from older basement rocks and (3) deposited the lead and fluorite without boiling.

Two-Dimensional Sheet Polymers Synthesized

The January 1, 1993, issue of *Science* contains a research article on the discovery of a synthetic pathway to two-dimensional polymers at the University of Illinois' Materials Research Laboratory (MRL) under BES/Materials Sciences support. A *Perspectives* article by a prominent Massachusetts Institute of Technology professor, Professor Edwin Thomas, in the same issue discusses the significance of this discovery. Professor Thomas calls attention to the fact that essentially all polymer molecules produced to date are basically one-dimensional objects. Now, Professor Sam Stupp and his group at the University of Illinois MRL have produced a two-dimensional sheet-like polymer object. Two-dimensional sheet polymers offer a number of obvious possibilities: ease of orientation, surface functionalization, tribological applications, and, as Professor Stupp indicates in his patent application, interesting nonlinear optical properties.

A key feature of these new materials is that they are both (in Professor Thomas' words) robust and flexible. Professor Stupp and his students have "produced the thin sheets by employing oligomers (short chain organic molecules) containing two different reactive sites: one site at one end of the oligomer and the other in the middle. The oligomers spontaneously self-organize into bilayers in solution. This locates one set of the reactive sites at the mid-plane thickness. Two independent, low-temperature reactions are then initiated and "stitch" the bilayer together via covalent coupling at the three bilayer levels. Even though the conversion of reaction sites is not 100 percent, there is sufficient redundancy created by the three layers of stitching that the bilayer is robust. The approximately

10-nm-thick sheets are very uniform in thickness, while their areal size is a function of the polymerization efficiency and the size of the preassembled oligomeric state. Many of the objects have areas of several square micrometers, corresponding to molecular weights of over 10^9 daltons."

Normally, high molecular weight materials have limited utility due to solubility and processing problems. These new materials do not have these limitations. The sheet-like molecules form a relatively low-viscosity liquid which can be readily processed into oriented films. More detailed understanding of the nature and properties of these new structures is needed before applications can become commercial but practical uses look promising. Moreover, the excitement in this discovery is the synthetic pathway to a two-dimensional architecture that can be expected to produce many types of organic materials with improved properties.

Technique Developed for the Analysis of Environmental Samples

Basic research of Office of Basic Energy Sciences/Chemical Sciences Division investigators Duckworth and McLuckey at Oak Ridge National Laboratory has led to the development of a new technique for the analysis of nonconducting samples of environmental interest, such as glasses and soils. This technique could prove important in the analytical requirements needed for remediation of DOE sites, e.g., the analysis of soil samples and the vitrification process. The development of a small, lightweight and easily field-portable instrument for environmental analysis is now practical. This new capability in analytical mass spectroscopy results from the first ever combination of a glow discharge source with a quadruple ion trap. Earlier reported work involved the development of a field-rugged system based on electron impact ionization of volatile organic compounds.

This amalgamation of glow discharge with a quadruple ion trap takes advantage of positive, complementary aspects of the two individual mass spectrometry techniques: glow discharge can be used to analyze nonconducting materials, and the ion trap can be used in the collisional dissociation of isobaric polyatomic ion clusters. This combination eliminates the interfering clusters that form during the analysis of nonconducting materials and extends the dynamic range of the technique.

Nuclear Magnetic Resonance Tomography Improves Characterization of Solids

A new type of nuclear magnetic resonance (NMR) tomography has been developed by researchers at Argonne National Laboratory under support from the Office of Basic Energy Sciences/Division of Chemical Sciences. The new technique simultaneously measures high-resolution NMR spectral information and resolves distances in the samples on a micron scale. The new imaging method uses a toroid cavity detector for rotating frame spectroscopy, and differs from conventional magnetic resonance imaging in that structural information is not lost during signal processing. Potential applications of this new technique would be in characterization of surface layers and in the production of advanced materials.

To solve the problem of sensitivity losses through magnetic coupling with metal pressure vessels, previous work by these researchers found that toroid cavity resonator detector probes had optimum magnetic flux confined to internal regions of the coil. Considerably greater sensitivity limits compared with conventional NMR detectors were demonstrated, and the new toroid probes have been granted a U.S. Patent.

The potential now exists for in-situ NMR investigations of reaction chemistry as a function of distance within the diffusion layer of electrochemical processes. A related advantage of the new approach to NMR imaging is that the toroid cavity probe may be inserted as a simple replacement for the standard detector in conventional Fourier transform NMR spectrometers.

AIDS and Buckyballs

Appearing in the August 2 issue of *Chemical and Engineering News* is an article on the activity of buckminsterfullerene against HIV-1 and HIV-2. Buckminsterfullerene, a soccer-ball (Buckyball) shaped molecule of 60 carbon atoms and whimsically named because of its similarity to the geodesic dome invented by Buckminster Fuller.

Buckminsterfullerene was discovered simultaneously in 1985 by two groups, one at Rice University and one in England. The Rice University group was and still is supported by Office of Basic Energy Sciences/Chemical Sciences Division for the study of the relationship between the structures and properties of metal clusters as models for chemical catalysis. The C_{60} discovery grew directly out of this work. At first, the interest was purely the unusual structure and chemical stability of C_{60}. It's hollow structure suggested that it could incorporate metal atoms and when such materials were prepared and studied they were found to be superconducting.

New methods have been discovered for making C_{60} in bulk quantities, furthering the study of possible applications. Most recently, scientists, noting the similarity of the structure of C_{60} to the structure of the HIV-1 protease enzyme, have used computer generated models to predict that C_{60} could bind to the enzyme blocking its active site. Experiments are now under way to evaluate the significance of this binding. This is another example of research driven by scientific curiosity that leads to potential new applications unforeseen at the time of the original research.

Materials Synthesis Using Biological Processes Highlighted

The October 1992 issue of the *MRS Bulletin*, published monthly by the Materials Research Society (MRS), contains the first of a 2-issue feature article on Biology and Materials Synthesis. The 2 issues discuss a newly emerging field of science in which biological processes are used or mimicked to synthesize new materials. The first issue features 6 articles, 3 of which concern work supported by the Materials Sciences Division and the Energy Biosciences Division in the Office of Basic Energy Sciences. The Guest Editor for these issues of the *MRS Bulletin* is Dr. M. D. Alper of the Lawrence Berkeley Laboratory who directs a project, Enzymatic Synthesis of Materials, which is also supported jointly by the Materials Sciences Division and the Energy Biosciences Division.

Structure of Northern California Revealed Using Teleseismic Images

Earth scientists at Lawrence Livermore National Laboratory and the U.S. Geological Survey have processed earthquake data from the CALNET array using techniques developed with funding from the Office of Basic Energy Sciences. The result is a 3-dimensional tomographic image of the rock velocity structure beneath northern California which provides a fundamental picture of the tectonic and volcanic processes in the region. The images reveal low velocity bodies identified as magma bodies associated with known volcanic fields such as the Clear Lake and Mt. Lassen systems. A low velocity body about 80 km north of Clear Lake may be an indicator of a newly forming volcanic field. The images also reveal the oceanic plate dipping steeply beneath the southern Cascade Mountains and northern Great Valley down to depths as great as 250km. These results provide a fundamental basis for understanding the interaction of tectonics, volcanics and earthquakes in the region as well as the foundation for applied research in resource evaluation and seismic hazards. The scientific team is being led by George Zandt, Earth Sciences Department, Lawrence Livermore National Laboratory, L-202 Livermore, California, and Harley Benz and David Oppenheimer, U.S. Geological Survey, Menlo Park, California.

Synthesis of Gallium Arsenide Quantum Dots Improved

Researchers supported by BES/Chemical Sciences Division have recently succeeded in synthesizing colloidal GaAs particles having a narrow particle size distribution (20 - 50 angstroms). These particles exhibit properties which makes them interesting as potential quantum dots. Quantum dot materials are of interest because of their unusual size dependant electronic, optoelectronic and photoredox properties. With normal materials these properties are composition dependant. However, with quantum dots these properties are dependant not on the material composition but on the size of the particle. Thus, the ability to tune the size through synthesis is a prime goal of the scientific community. The synthetic route developed by B. Curtis and A. Nozik at the National Renewable Energy Laboratory (NREL) utilizes the organometallic chemistry of As and Ga to produce small colloidal gallium arsenide particles. With III-V semiconductors the principle problem has been in devising synthetic routes with sufficient selectivity to yield a clean product with a small particle size distribution. The advance by the NREL group is in matching the organometallic precursors with the coordination power of the solvent to control the growth of the particles. The objective of continuing studies is to understand how both the absolute size and the size distribution can be controlled so that particles of any size can be made with a distribution of only a couple of angstroms. Such particles could be the basis for new non-linear optics, new optical computers and/or solar photocatalysts.

Researchers Observe First Band Gap Narrowing in Ordered Compound Semiconductor

The National Renewable Energy Laboratory recently reported the first observation of band gap energy reduction ("band gap narrowing") in the compound semiconductor $Ga_{0.47}In_{0.53}As$. In a project funded by Basic Energy Sciences/Materials Sciences, Drs. D. J. Arent, M. Bode, K. A. Bertness, S. R. Kurtz, and J. M. Olson found that samples of $Ga_{0.47}In_{0.53}As$ grown epitaxially on (100) InP which exhibited ordering into the CuPt crystal structure had a reduction in band gap energy, whereas samples which did not exhibit such ordering did not have an energy reduction. Studies of the dependence of band gap narrowing on growth temperature and deposition rate for $Ga_{0.52}In_{0.48}P$ and $Ga_{0.47}In_{0.53}As$ suggest that similar mechanisms are controlling the narrowing for these two materials and imply the criteria to apply in unexplored growth regimes and materials systems. The band gap narrowing induced by the ordering allows an additional degree of freedom in optimizing properties for possible applications in solar cells, detectors, and long wavelength lasers.

High Temperature Plasticity of Solids Explored in Workshop

The BES/Division of Materials Sciences Sponsored a Workshop on "Grain Boundary and Interface Phenomena in the High Temperature Plasticity of Solids" in Oakland, California, during October 12-16, 1992. The purpose was to identify research needs and opportunities in the understanding of the role of interfaces in the elevated temperature mechanical behavior of advanced materials in which interfaces are significant. The materials include: nanostructures, ceramic matrix composites (CMC) and superplastic ceramics and metals. Participants included 24 persons, 7 from the Department of Energy laboratories, and 14 from universities. Three foreign scientists attended, two from Japan and one from the United Kingdom. The important findings included: (1) a need for improved understanding of the relation between grain-boundary structure and the sliding/cavitation propensity, (2) a need for improved materials and experiments to determine the mechanical-properties/microstructure relationships in nanostructures, (3) an understanding of the basic deformation mechanisms of new, high-strain-rate, superplastic materials, (4) the need to understand the basic role or low-misorientation interfaces on 3 and 5 power-law creep plasticity in traditional and advanced materials, and (5) understand the slip processes at the matrix/fiber interfaces in CMCs. The proceedings of this workshop will comprise a future issue of the refereed journal, *Materials Science and Engineering*. The co-chairpersons were Dr. M. E. Kassner, a detailee from Lawrence Livermore National Laboratory to the Office of Basic Energy Sciences/Division of Materials Sciences and Professor T. G. Langdon of the University of Southern California.

Materials Research Benefits from Complexity

The October 1992 issue of *Physics Today* contains a special emphasis on "Complexity and Materials Research." It is now clear that consideration of more complex materials provides a new window of opportunity in terms of new materials with novel or improved physical properties. This issue contains five articles on forefront activities in materials, including two authored by Basic Energy Sciences/Division of Materials Sciences grantees. They are James

S. Langer of the University of California at Santa Barbara writing on "Issues and Opportunities in Materials Research," and Leo M. Falicov of the Lawrence Berkeley Laboratory writing on "Metallic Magnetic Superlattices."

Aging of Energy Production and Distribution Systems Examined

The Proceedings of the workshop on *Aging of Energy Production and Distribution Systems* that was held at the Rice University on October 11-13, 1992, have been published in a special issue of the *Applied Mechanics Reviews* (Vol. 49, No. 5, May 1993, The American Society of Mechanical Engineers, New York.) The workshop was sponsored by the Engineering Program, Office of Basic Energy Sciences/Division of Engineering and Geosciences, to identify the basic research issues related to reliability and life prediction/life extension of aging energy related structures. The Proceedings include papers presented during the workshop. They are divided among eight sessions, FOSSIL FUEL PLANTS, NUCLEAR POWER PLANTS, OFFSHORE PLATFORMS, DISTRIBUTION SYSTEMS, MATERIALS, STRUCTURES, INSPECTION AND MONITORING, and ASSESSMENT. While the first four deal with the issues related to specific industrial facilities, the last four address generic basic research needs. In addition to the papers each session concludes with a summary prepared by the chair of the session resulting from the discussions among the speakers and other participants. The Proceedings will be helpful in stimulating appropriate proposals for future research in aging of energy related structures.

Research Needs Identified for Highly Conducting Ceramics

The Materials Sciences supported workshop "Research Needs and Opportunities in Highly Conducting Electroceramics" has been published as a Special Review in Materials Science and Engineering (B18, 1993, pages 52-71). The 25 contributors to this workshop included 14 from universities, 5 from the Department of Energy laboratories, 4 from private industry, 1 from Canada and 1 from the Materials Sciences Program. Electroceramics includes ceramics that are classified as electronic conductors, ionic conductors, mixed (electronic/ionic) conductors, and insulators. Taken collectively, they exhibit electrical conductivity from less than 10^{-16} Seimens per meter to 10^{8} Seimens per meter, or a range of 24 orders of magnitude. A few of their myriad applications include sensors, electrodes, heating elements, solar cells, catalysts, solid oxide fuel cells, solid-state batteries, ion selected membranes, electronic packaging and substrates, thermistors, varistors, and switches. The needs and opportunities that were identified and discussed included modeling of electronic transport processes including quantum mechanical modeling techniques and a methodology for treating conduction in highly detective crystalline materials, and glasses, understanding defect chemistry, defect interactions, charge transport and reaction mechanisms at and along interfaces and grain boundaries, and advanced synthesis and processing methods such as for nanostructured materials, thin films, composites, and modulated structures. This workshop was organized and chaired by Dr. William J. Weber of Pacific Northwest Laboratory, who is on a quarter-time assignment to Materials Sciences and was co-chaired by Professor H. L. Tuller of Massachusetts Institute of Technology, T. O. Mason of Northwestern University, and A. N. Cormack of Alfred University.

Review Series Being Published in Electrochemistry

Dr. Philip N. Ross, Lawrence Berkeley Laboratory, along with Dr. Jacek Lipkowski of the University of Guelph, Canada, has initiated a new series of review volumes entitled, "Frontiers of Electrochemistry". The first volume, "Adsorption of Molecules at Metal Surfaces," has just appeared in print. Volume two, "Structure of Electrified Interfaces," is in press and volume three is approximately one-half finished. The new series, which emphasizes the physics and chemistry of electrochemical systems, is one of only two review series in the field.

Cubic Boron Nitride Film Deposited on Silicon Substrates

A research team at Sandia National Laboratories, Livermore, has prepared boron nitride films containing up to 85% cubic boron nitride (cBN). Cubic BN has a crystal structure analogous to that of diamond and is somewhat harder than diamond. The Sandia team found that ion-bombardment of the silicon surface was necessary to promote the preferential formation of cBN films. A laser beam from a pulsed excimer laser evaporated the hexagonal boron nitride (hBN) source, and the vapor plume impinged on a silicon substrate heated to 400°C. An ion beam consisting of a combination of Ar and N_2, with a beam energy between 100 and 1200 eV, irradiated an area of the substrate. Infrared reflection spectroscopy, high resolution transmission electron microscopy and selected area electron diffraction were used to determine the composition of the film. This work was performed by T. A. Friedman, K. F. McCarty, E. J. Klaus, H. A. Johnsen, D. L. Medlin, M. J. Mills, D. K. Ottesen and R. H. Stulen on a project supported by the BES-Materials Sciences Division.

Photo-Induced Changes Observed in Magnetic Materials

Scientists at Argonne National Laboratory and the University of California, San Diego, have observed an unexpected photo-induced change in the interlayer magnetic coupling of iron - iron silicide superlattices, a class of superlattices which exhibit several interesting and potentially important magnetic characteristics. Indirect magnetic exchange coupling is observed between the iron magnetic layers across intervening nonmagnetic iron silicide layers. This coupling aligns the adjacent magnetic layers in either a ferromagnetic or antiferromagnetic configuration, depending on the thickness of the nonmagnetic spacer. As the spacer thickness increases, the coupling oscillates in sign from ferromagnetic to antiferromagnetic with a nanometer-scale periodicity that depends on the properties of the spacer metal.

The samples used in this investigation exhibit antiferromagnetic coupling at room temperature which become ferromagnetically aligned when cooled below 100 Kelvin. However, the antiferromagnetic coupling can be restored at low temperature by exposure to visible laser light. This appears to be the first example of such photo-induced changes in the interlayer coupling of magnetic superlattices. The implications of the results are that both thermally and photo-generated charge carriers in a silicide layer are capable of communicating spin information from one magnetic layer to the next; the silicide coupling medium is identified as a small-gap semiconductor (an observation with theoretical consequences).

The discovery points the way towards atomically engineered magnetic and optical properties via band-gap tailoring of the semiconducting spacer layer. The work offers renewed promise of integrated semiconductor and magnetic materials to create new optoelectronic and photomagnetic devices.

New Semiconductors Help Generate High Efficiency Laser Light

The semiconductor laser was first demonstrated in 1962 and has undergone extensive research and development to its present day form. It is compact, rugged, and highly efficient. Because of these reasons, the semiconductor laser is finding many new applications. However, these lasers suffer from the fact that the lasing beam is not very well controlled. The beam spreads widely as its travels, so the concentration of power is degraded. Worse, the beam is nonuniform, having bright and dark areas. To overcome these problems, future generations of lasers will require new semiconductor materials which are engineered to control light emission. Dr. Paul L. Gourley and colleagues at Sandia National Laboratories/Albuquerque, under a BES/Division of Materials Sciences program, are examining a new class of semiconductor materials called photonic lattices designed to harness light by the efficient generation of narrow, uniform beams.

For the first time, experimental confirmation of high efficiency lasing in a semiconductor photonic lattice has been obtained. This effect was observed in photonic lattices fabricated by etching periodic microscopic cells (approximately one tenth the thickness of a human hair) in a semiconductor microcavity crystal grown by molecular beam epitaxy. The crystal comprises hundreds of layers of compound semiconductor materials grown with atomic precision. When the lattice is energized by light from a separate pump laser, it lases with high efficiency and emits a narrow, well-controlled beam. Most striking was the observation that the pump power required to achieve lasing did not increase as larger and larger areas of that lattice were energized. This shows that a large lattice uses the generated light more efficiently than conventional semiconductor lasers. When the lattice area became very large (larger than the cross section of a single human hair), the pump power required for lasing approached the theoretical limit for high efficiency lasing from a photonic lattice.

Patent Filed on Novel Hydrogen Storage Materials in United States and Japan

A patent on an invention using cluster ions as hydrogen storage materials has been filed in the United States and Japan by the Center of Innovative Technology in Virginia on behalf of the Virginia Commonwealth University. The Center of Innovative Technology sent this patent application to the National Institute of Standards and Technology for evaluation. The initial evaluation rated this invention in the top 5%, and it is undergoing indepth study. Office of Basic Energy Sciences/Materials Sciences Division grantees Professors P. Jena and B. K. Rao of Virginia Commonwealth University made a surprising theoretical prediction that one positively charged metal ion (e.g., Ni^+) can bind as many as 10 hydrogen molecules in a *Physical Review Letters* article; this was the first prediction of molecular chemisorption to a transition metal ion. Subsequently, this prediction received experimental confirmation by Professor Michael Bowers of the University of California at Santa Barbara. This new concept is important in the search for environmentally safe storage of energy.

Also, Professor Jena was chosen to receive Virginia Commonwealth University's highest honor—the Award of Excellence—for 1993 in a special convocation on February 10, 1993. This award recognizes his superior performance in teaching, scholarly activities and services. He was praised for his pioneering work on atomic clusters, for organizing many highly successful international symposia, and for services to his profession and community.

Aqueous Biphasic Separation Process Subject of Patent

The ARCH Development Corporation, established to aid in the commercialization of ANL inventions, has filed a patent application for an Aqueous Biphasic Separation (ABS) process that was developed in the Chemical Technology Division. The invention makes use of ABS systems for the separation and recovery of submicron-sized particulates. The ABS process has applications in the separation and recovery of plutonium from defense wastes and in the decontamination of soils. The separation process involves the selective partitioning of submicron particulates between two immiscible phases. Colloid-size particles that are suspended in an ABS system will partition to one of the aqueous phases, depending on a complex balancing of particle interactions with the surrounding solvent. ABS systems are ideally suited to waste treatment applications because the primary component is water. In addition, the water-soluble polymers that are used in biphase formation are inexpensive, nontoxic, and biodegradable. Besides the application to radioactive wastes, the patent also covers the use of the ABS process for the separation of submicron-sized quartz particles from kaolin clay. This invention opens the way for commercial utilization of certain high grade ore deposits found in the U.S. and Mexico. The work is being supported by the Office of Basic Energy Sciences/Division of Advanced Energy Projects. Dr. David J. Chaiko of ANL is the Principal Investigator.

Energy Radiation from Seismic Sources Mapped

Researchers at The University of Southern California have developed a new method for analyzing seismic data from earthquakes. The method maps the high frequency energy radiation on the earthquake fault plane and identifies not only the energy release but also the direction of motion and the block size involved in such motion.

The method was applied to the Loma Prieta earthquake (M=7.1, October 17, 1989) and identifies three concentrations of energy release over a 20 km long segment of the fault. The central concentration is located near the earthquake hypocenter; the northwest concentration is associated with along strike motion and the southwest concentration is associated with dip motion. These observations suggest that the high frequency energies are radiated from the boundaries of the large slip zones. The results support theoretical considerations that high frequency waves are primarily generated from the rupture stopping areas and places of large slip variation. These results thus define the block size and block motion responsible for this earthquake and provide a new basis for understanding, engineering and mitigating earthquakes.

When applied to smaller scales, this new method can also serve as a diagnostic for hydrofracturing in reservoir extraction enhancement, safety evaluation in mine engineering and remote techniques for energy and environmental excavation. This research was supported in part through a grant provided by the Office of Basic Energy Sciences/Division of Engineering and Geosciences.

New Ionization Techniques for Liquids Expands Utility of Mass Spectrometry

Basic research by Texas A&M University investigators in mass spectrometric analysis have developed a new technique for liquid sample introduction and ionization. The Texas A&M group, supported by the Office of Basic Energy Sciences/Division of Chemical Sciences, has developed an aerosol based matrix-assisted laser desorption ionization (MALDI) technique for liquid samples. This novel technique was predicated on basic research in matrix-assisted laser desportion ionization which involved samples mixed in a solid matrix. The solid matrix method has been extended to liquids for the first time by aerosol generation from a solvent stream containing the matrix element dissolved in it. The aerosol is desolvated during introduction to the mass spectrometer and the dry microcrystalline particles produced behave as the matrix when exposed to the laser beam. The sample molecule is ionized and desorbed from the microcrystal and then analyzed in the mass spectrometer. The advantages of this new introduction and ionization technique are the higher liquid flow rates addressable with this system (which is important in liquid chromatography-mass spectrometry) and the ability to ionize large peptides and biomacromolecules. This new technique could prove useful in the Department of Energy's continuing efforts in waste characterization and remediation.

Superheating and Repairing a Metal Surface

The August 26, 1993, issue of *Science News* contains an article with the above title in which theoretical work has confirmed that a close packed metal surface can be heated considerably above the metal's bulk melting temperature without melting in spite of the presence of defects in the surface layer. Uzi Landman of the Georgia Institute of Technology, whose theoretical research is supported by Materials Sciences, points out in an August 16, 1993, article in *Physical Review Letters* that this result is surprising since defects have long been viewed as the cause of melting. Landman was inspired to simulate the response of a close packed metal surface to intense laser pulses due to research published last year which experimentally demonstrated that a close packed lead surface could be heated 120 Kelvins above the bulk lead melting temperature without the onset of melting. This experimental work by Elsayed-Ali at Old Dominion University was also supported by Materials sciences and has received considerable attention in both scientific and popular press accounts. Elsayed-Ali has shown that this superheating is a rather general phenomena.

Neutrons "See" Polymer Motion

Understanding diffusive transport in polymers is important in many polymer applications. For instance, the strength of a "weld" between two polymer components depends upon the distance over which the two components mix or intertwine via their motion. The most widely accepted theory to explain these phenomena has been the reptation model of Nobel Laureate P. G. deGennes. DeGennes pictures the chains moving in a polymer as if they were a basket of snakes (hence the term "reptation"). Each of the snakes is highly entangled with its neighbors and must move in a convoluted path along its length.

Scientists at Argonne's Intense Pulsed Neutron Source (supported through the Office of Basic Energy Sciences/ Division of Materials Sciences) have found the first direct verification that polymer chains reptate. While this result does not yet confirm the deGennes theory in detail, the results provide an important test for all theories of polymer diffusive transport.

By selectively labeling two polymers by replacing hydrogen with deuterium at certain locations, e.g., the polymer ends, samples for depth profiling were made. In these samples, the interface between the two polymers is invisible unless the chain ends and centers diffuse across it at different rates. If the molecules move along their contours, then the ends must go first. With both high resolution neutron reflection and lower resolution secondary ion mass spectrometry, the interfacial profile was observed to change during the polymer motion from invisible, to a shape characteristic of the polymer ends moving faster than the centers. This is understood in terms of the reptation model since once the polymers have diffused a distance comparable to their own length, then any inhomogeneity of movement at smaller length scales would no longer be visible.

These results, with no indirect interpretation or modeling necessary, directly show that polymers move "head first" along their contours. By repeating these experiments with different lengths of polymer chains, the reptation model can be critically tested and a major contribution will be made to the understanding of diffusive transport in polymers.

Collaborators in this research include: W. D. Dozier and G. P. Felcher of Argonne National Laboratory, T. P. Russell and V. R. Deline of IBM, and G. Agrawal (advisor: R. P. Wool) of the University of Illinois.

New Condensation Reaction Found for Production of Nitriles

The production of nitriles is important because they are industrial chemicals used as starting materials for polymers, pharmaceuticals and pesticides. Researchers at Louisiana State University have found a new synthesis for their production. The synthetic route involves chain condensation of alkylamines which results in dimerization of the hydrocarbon chain and conversion of the alkylamine groups(CHx-NH2) to nitrile groups (CN). This reaction was found to occur in a Cu-zeolite catalyst that has been studied by this group. Professor Price has been supported by the Office of Basic Energy Sciences/Chemical Sciences Division for this work. A patent application has been filed for the catalyst and the process for converting amines to nitriles.

Helium-Irradiation Found to Remove Copper Impurities from Silicon

In laboratory experiments funded initially by the Office of Basic Energy Sciences/Division of Materials Sciences, Samuel Myers, Dawn Bishop, and David Follstaedt of Sandia National Laboratories/New Mexico, have demonstrated that voids introduced into silicon by helium irradiation can serve as effective gettering surfaces for the removal of copper impurities. Metals such as copper degrade the performance of silicon-based microelectronics. The researchers formed the voids by irradiating a silicon crystal with helium ions and then heating the silicon to drive off the helium and to grow nanometer size voids. Since the helium-ions deposit their energy only in the region of the material where they are finally stopped, a large portion of the crystal is left undamaged by the irradiation, and voids are localized in a narrow band in the crystal. To investigate the removal of copper, copper was introduced into a silicon sample by ion-implantation, and the sample was heated to investigate its removal of the voids. Myers and his colleagues found that the attraction of the voids for the copper was so great that copper was removed until the surfaces of the voids were coated. The group is investigating the gettering action of the voids for other metals.

High Temperature Deformation Processes in Metals and Ceramics Published

The proceedings of an Office of Basic Energy Sciences Workshop "Grain Boundary and Interface Phenomena in the High Temperature Plasticity of Solids," were published as a 243 page dedicated issue of *Materials Science and Engineering* on July 15, 1993. The subject is a critical one in terms of our understanding and control of high-temperature deformation processes in metals and ceramics. The latter in turn is of paramount importance to reliable long-time high-temperature load bearing capability in structural metals and ceramics and to ultra-high rate deformation processes utilized in the low-cost fabrication and manufacture of sheet metal products. The Workshop identified research needs, opportunities, and technological barriers to be overcome in five key areas: grain boundary design, nanocrystalline solids, processing, superplastic deformation, and ceramic matrix composites. This Workshop was organized and the proceedings were edited by Dr. M. E. Kassner, who is on part-time assignment to the Division of Materials Sciences from Lawrence Livermore National Laboratory, and Professor T. G. Langdon, of the University of Southern California. The invited participants were drawn from universities, national laboratories, private sector industry and abroad.

Highest Sensitivity Achieved for Capillary Absorbance Detection

Basic research by Ames Laboratory chemists on methods of sensitive detection in capillary electrophoresis for micro-analytical separations has resulted in an enhanced absorbance detector. The key to the general applicability of this method lies in the sensitive detection of minute quantities of analyte molecules. The Ames group, supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, has developed an on-column double-beam laser absorption detection technique for molecular species at the 45,000-molecule level. This is the most sensitive known direct absorbance detection method for capillary electrophoresis. This new detector could prove flexible enough to be of general use for both capillary electrophoresis and capillary liquid chromatography. Capillary electrophoresis is rapidly growing in importance in the separation field and is based upon the migration of charged molecules in a capillary tube, typically 100 μm or smaller in diameter. The Ames group has been using this technique to separate the components from single red blood cells at detection limits previously unattainable.

Photo-Induced Reactions on Semiconductor Surfaces Examined

The existence and role of hot-electron chemistry has been a subject of interest for many years in semiconductor electrochemistry where the tunneling of hot electrons through a surface barrier is of technological importance. The dynamics of such processes have recently become amenable to experiment through use of photochemical techniques. In recent experiments by R. Osgood of Columbia University, with support from both the Chemical Sciences and Material Sciences Divisions of the Office of Basic Energy Sciences, it has been shown that hot-electron chemistry is an important mechanism on semiconductor surfaces, a conclusion made possible by the translational energy resolution of the experiment on a well-defined gas-solid interface.

Semiconductor Technology for High Temperature Superconductors

Recent studies were conducted by Dr. Moreland of the National Institute of Standards and Technology supported by the Office of Basic Energy Sciences/Engineering Research program on thin films of a high temperature superconductor (YBCO) and semiconductor devices deposited on yttrium stabilized zirconia-buffered silicon (Si). Scanning tunneling microscopy and atomic force microscopy revealed pinholes in the yttrium stabilized zirconia films which vary in size (5-44 nm). This is the first direct proof of the presence of such defects. Ideally the buffer layer should be continuous in order to prevent chemical reaction between YBCO and Si. Atomic force microscope images of the completed bilayers show scattered mounds having about the same surface density as that of the pinholes. This suggests that the YBCO reacts with Si during the high temperature processing steps to form nonconducting phases near the pinhole sites. Atomic force microscope images also show large "boulders" on YBCO films, a result of the laser ablation process, and microcracking in etched YBCO layers. These features would adversely affect the critical temperature and current of films. The information gained from scanning tunneling microscope and atomic force microscope studies will help researchers optimize the transport properties on narrow YBCO lines on Si.

Improved Method for Electromagnetic Imaging of Reservoirs

Scientists from Lawrence Berkeley Laboratory and the University of California-Berkeley, supported by the Office of Basic Energy Sciences/Geosciences program, have developed a mathematical formulation of the low frequency, diffusive electromagnetic fields suitable for tomographic inversion of electromagnetic data. Numerical experiments show that the formulation is capable of accurately extracting the position and attitude of target fractures. These results pave the way for extended crosshole electromagnetic tomographic imaging in reservoirs.

The location of fractures is an important aspect of reservoir characterization because fractures constitute the major pathways for reservoir fluids. Although seismic methods can be used for this purpose, the elastic wave velocity contrast between fractured rock and non-fractured rock is small. On the other hand, fluid filled fractures differ by orders of magnitude in electrical conductivity from the surrounding rock thus making EM detection of fractures potentially quite useful.

Photochemical Energy Conversion Achieved in Zeolite Assemblies

Long-lived photoinduced charge separation has been achieved in zeolite assemblies. In research performed by Professor Prabir K. Dutta of Ohio State University and supported by the Office of Basic Energy Sciences/Division of Chemical Sciences, the novel architecture of the zeolite framework structure has been exploited for organization and separation of the components of an artificial photosynthetic assembly. As reported in *Nature*, polypyridyl ruthenium photoactive molecules entrapped in zeolite supercages interact through windows of the cage with relay molecules in neighboring cages, which subsequently transfer electrons to acceptor molecules in the surrounding solution medium. The appealing aspects of this model system, as compared to other strategies currently being investigated for charge separation by multicomponent assemblies, are the slow back reaction and ready accessibility of the photochemically generated products.

Argon Plasma Deposition Process Found to be Highly Sensitive to Contaminants

Partially ionized argon, or argon plasma, at near atmospheric pressure is useful as a carrier medium for the deposition of hard coatings on soft substrates. Such a plasma is known to be in a partial local thermal equilibrium. That knowledge has served as a basis for the interpretation of some standard diagnostics for the control of the deposition process.

However, research carried out by Professor Kruger (Stanford University) sponsored by the Office of Basic Energy Sciences/Engineering Research program shows that small levels of contamination of argon plasma by hydrogen and/or nitrogen prevent the use of some standard diagnostics for process control. For example, measurements of light emission from an argon plasma containing as little as 0.2% of hydrogen indicate apparent but not real temperature readings which are higher than achievable under the experimental conditions, indicating that even small quantities of the diluent throw the system out of partial thermal equilibrium. Similar results have been found for small additions of nitrogen. This research effort shows unequivocally the need for more sophisticated approaches to the interpretation of data used in the control of plasma processing of materials.

Superconducting Transport Properties Investigated

Oak Ridge scientists supported by the Office of Basic Energy Sciences in collaboration with J.M. Phillips of American Telephone and Telegraph Bell Labs have used highly controlled, pulsed currents to investigate dissipative superconducting properties at exceptionally high power levels. Although the phenomenon of superconductivity is often associated with a state of vanishing resistance, this is neither a necessary nor sufficient condition for characterizing the superconducting state. At current densities beyond the critical value (critical current) dissipation sets in - although superconductivity itself persists up to a higher level known as the pair-breaking current. Novel and interesting physics is expected to occur between the critical current and the pair-breaking current, and some of these effects have been investigated.

One such effect is the process of free-flux flow, as described by the Bardeen-Stephen model, whereby the ratio of the free-flux flow to normal-state resistivities is simply related to that of the magnetic flux density and upper critical field. Measurements on thin films of copper oxide high temperature superconductors have provided the first verification (in any superconductor) of this very basic phenomenon. Another experiment just completed, investigates the pair-breaking effect of a high current (not seen before in any high-temperature superconductor) and thus deduces the temperature dependence of the pair-breaking current. Excellent agreement was obtained with the behavior predicted by Ginzburg-Landau theory.

Both results are of pivotal significance in understanding the phenomenon of high-temperature superconductivity. The work on flux-flow shows the conventional nature of the mixed state - a topic that has been filled with controversy and confusion. The second result on the pair-breaking effect serves to lay crucial groundwork at a time when the theoretical understanding of high-temperature superconductivity is still under development. It shows that some of the traditional concepts about the formation of the superconducting state are applicable to high-temperature superconducting materials as well.

Transport of Solvents in Polymer Networks is Better Understood

Magnetic resonance imaging (MRI), a spectroscopic technique, is providing a new window into the transport of solvent molecules in polymer networks. By MRI mapping the migration of solvents through various polymer specimens, researchers Robert Botto and George Cody of Argonne National Laboratory are able to distinguish between different modes of transport behavior associated with fundamentally different types of polymer systems. The research is supported by the Office of Basic Energy Sciences/Division of Chemical Sciences and the understanding of these transport phenomena is of great importance to many industrial and biological processes such as film coating and casting, developing of solvent-resistent polymers and photoresists, design of drug delivery systems, and upgrading of fossil fuels.

Geochemistry "Perspective Article" Published in *Science*

Professor Alexandra Navrotsky of Princeton University is the author of an article about the geochemistry of the earth's mantle in the July 9, 1993, issue of *Science* magazine. A thermodynamic perspective of geochemistry provides one of the keys to understanding the mineral formation and dynamic processes within the interior of the Earth. The distribution of petroleum and geothermal sources have obvious importance for the Department of Energy. The research methods for studying material behavior under the severe conditions of temperature and pressure are also applicable to material performance under the demanding conditions of energy production and use.

For the case of the Earth's interior, as Professor Navrotsky points out, an understanding of the thermodynamic behavior of magnesium and iron silicates provides insights into the probable material transformations which occur at the major discontinuities within in the Earth, such as the Mohorovicic discontinuity (or Moho), between the crust and the upper mantle and the much larger discontinuity between the lower mantle and upper core. But, many questions remain to be answered. For example, little is known about the nature of hydrous crystalline forms (minerals containing chemically bound water) that might exist within the mantle.

For her research on energy-related materials, Professor Navrotsky receives her support from the Office of Basic Energy Sciences/Division of Materials Sciences for the study of the energetics of phases related to oxide superconductors, and from the Division of Engineering and Geosciences on thermodynamic properties of geologic materials.

"When Theory has the Confidence to Challenge Experimental Data"

The above quote is the title of an article in the May 1993 issue of *Science Watch* that discusses the current compilation of the ten most cited papers in chemistry. The theoretical paper referred to in the quotation is entitled "GAUSSIAN-2 theory for molecular energies of first- and second-row compounds." The lead author is Dr. Larry Curtiss of Argonne National Laboratory; his collaborators are two theorists from the American Telephone and Telegraph Bell Laboratories and a Professor from Carnegie Mellon University. Dr. Curtiss' research at Argonne is supported by Materials Sciences.

The cited paper describes the results of a long-standing research program to produce a highly accurate method for calculating various molecular energies. Reported in the paper are calculated values of a number of molecules and molecular ions. Exceptionally good agreement was found with published experimental values for many of the calculated species. However, for a significant number, the calculated values were way off the reported experimental values. The theorists were sufficiently confident of their method to challenge the published experimental data. As a result of the published theoretical work, a number of systems have been experimentally reexamined (the experiments are difficult) and in all cases studied, the revised experimental results agree very well with theory.

Technique Developed for the Analysis of Organic Solution Residues

Research supported by the Office of Basic Energy Sciences/Division of Chemical Sciences at the Oak Ridge National Laboratory has lead to the development of new, simple, and efficient methodology for the analysis of contaminant metals in organic residues using Glow Discharge Mass Spectrometry (GDMS). GDMS has been used to analyze solid samples directly, but solutions containing organic substances, e.g. oil, have necessitated the development of a simple sample preparation scheme using a low temperature ashing step. The organic solution is mixed with a silver powder, ashed to remove the organics, and the metal-containing residue pressed into a glow discharge electrode. Preliminary experimental results for the determination of lead in a standard reference oil have shown GDMS to be comparable to the method approved by the Environmental Protection Agency for these complex sample matrices. This GDMS technique could enhance sample throughput in the characterization of waste sites due to the minimal sample preparation needed as compared to other analytical techniques.

Solid State Nanostructure Technology Featured in *Physics Today* Series

The June 1993 issue of *Physics Today*, a monthly publication of the American Institute of Physics, is a special issue in which all six scientific articles concern the optics of man-made semiconductor nanostructures (artificial structures whose chemical compositions and shapes are controlled with nanometer accuracy). This special issue was organized by Professor Daniel S. Chemla, Director of the Materials Sciences Division, Lawrence Berkeley Laboratory, and Professor of Physics at the University of California at Berkeley. Professor Chemla also authored an article on nonlinear properties of low-dimensionality materials when probed by intense or very short light pulses. This series of articles highlights the ability of modern technology to make solid state nanostructures that have the potential for revolutionary applications in electronics and optoelectronics. Professor Chemla's research is funded by the Office of Basic Energy Sciences/Division of Materials Sciences.

Transmission Electron Microscopy Elucidates Mineral Disorder

Crystal defects and chemical reactions occurring at scales beyond the resolution of light microscopes have major effects on the chemical and physical properties of rocks and minerals. High resolution imaging and chemical analysis well below the 1 nanometer scale with analytical spatial resolution approaching 10 nanometers define important new methods for exploring reaction mechanisms and kinetics of natural processes. A synthesis of ongoing research in this field is reported in *Science* by a collaboration of scientists led by David R. Veblen and including 4 scientists from universities and national laboratories supported by the Office of Basic Energy Sciences/Division of Engineering and Geosciences. Their results have established that (1) structural disorder is common in some minerals and rare in others, (2) many mineral reactions are controlled by atomic cluster scale mechanisms and (3) submicron inclusions and intergrowths significantly influence solid state reactions.

This research opens a frontier in the atomistic understanding of the controls on the mineralogic record left by multiple Earth processes; it allows elucidation of the complex interplay between aqueous chemistry, surface reactions, silicate melt formation, phase transitions and deformation. These processes are in many ways analogous to processes of interest to materials scientists and solid state physicists. New endeavors in atomistic level geologic materials research will provide a detailed record of Earth processes occurring over environmental and geologic time and space scales. In addition, such research will provide a host of experimental conditions and time scales for materials research not available for laboratory study.

Silicate Minerals Exhibit Low Diffusion Rates

Solid state internal diffusion at low temperatures is a particularly important limiting condition in the analysis of geologic mass transport. Diffusion and coupled diffusion data are essential in the analysis of important interactions at mineral interfaces as related to geothermal, nuclear waste disposal, and contaminant transport problems. Drs. R. T. Cygan and C. S. Schwandt at Sandia National Laboratories, Albuquerque, have used resistive evaporation of metal oxides on garnets to prepare thin-film diffusion couples used in measurement of diffusion coefficients and estimation of activation energy. Depth profiles were obtained using an ion-probe at the Sandia-Los Alamos-University of New Mexico facility. Self-diffusion coefficients for magnesium and calcium were determined for various garnets at temperatures from 800 degrees to 1000 degrees Celsius at a range of oxygen pressures. Magnesium diffusivity on the order of 10^{-22} meter^2/sec were found at 800 degrees Celsius for the types of garnet called pyrope, some 4 orders of magnitude less than estimated from previous high temperature extrapolation. The direct measurement of these very low diffusivities provides the foundation for a new perspective on diffusion in silicate minerals under geologic conditions. The investigators are now assessing the lower temperature limits for obtaining direct diffusivity measurement using the ion probe technique.

Droplet Size Distribution in Fragmentation of Liquid Filaments

In controlling many processes, it is useful to know the distribution of droplet sizes arising from the breakup of liquid filaments. Intuitively, it is obvious that droplets are most likely to form around the neck of a deformed filament. It is less obvious that droplets formed in this fashion are inevitably accompanied by smaller satellite droplets.

A study of the filament fragmentation process carried out by Professor J. Ottino at Northwestern University, supported by the Office of Basic Energy Sciences/Engineering Research Program, revealed the precise nature of the mechanism which produces the satellite droplets: as the neck in the filament narrows and eventually tears, the strands attached to the bulk of the filament and left behind on either side of the newly formed drop break up further before surface tension can pull them back to the body of the filament. Each of the resulting smaller drops is accompanied by two satellite drops, and so on. Computations based on this mechanism are in good agreement with experimental data.

The results of this study will help explain how very viscous fluids are fragmented and dispersed in the flow of less viscous liquids.

Smoothing Kinetics on a Rough Surface

Molecular beam epitaxy is a technologically important technique used in the growth of multilayer semiconductor systems and metal overlayers on semiconductors. It is intended to grow smooth layers, which is achieved after the empirical determination of suitable deposition rates and temperatures. A substantial body of theoretical work has examined the mechanisms by which a smooth layer develops, but experimental work has been extremely limited. To study the smoothing phenomenon directly, J. K. Zuo of Southwest Missouri State and J. F. Wendelken of Oak Ridge National Laboratory used high-angular resolution, low-energy electron diffraction to observe the smoothing kinetics of a rough surface prepared by the epitaxial deposition of copper on copper (100) to produce a multilayer terrace type of structure. The results verify a theory which predicts that the smoothing rate for this type of structure is controlled by an evaporation-condensation mechanism which is a function of the curvature and separation of the atomic step edge.

The measurements examine both the development of the roughened surface and the subsequent smoothing. Copper was deposited at room temperature on an initially smooth (100) surface having a step separation of about 550 A. Square islands developed in the first atomic layer but with the deposition equivalent of 100 atomic layers, the surface could be described as a multilevel terrace structure with an average terrace width of only 35 A. Upon heating this surface quickly by 30 degrees to 60 degrees celsius, smoothing was observed to occur via observation of the changing lineshape of a diffracted electron beam. The smoothing displayed a power law dependence on time, with a rate initially proportional to the one-third power. Comparison with published theories for the smoothing phenomenon indicates that the driving force for smoothing is the line tension difference of step edges with different curvatures, which results in the removal or evaporation of atoms from terrace edges with small radii and their subsequent relocation to terrace edges with larger radii. Also predicted by theory, scaling was observed during this smoothing (i.e., it was observed that the terrace width size distribution function remained the same while the average length scale increased). After the average terrace widths grew to an average size of 200-250 A, the smoothing slowed to be proportional to the one-fifth power of time, and the scaling behavior broke down. While some theories indicate this to be expected for a diffusion limited situation, surface entropy, which is expressed as a steady-state roughness, may also be a limiting factor.

Surface Crystallization of n-Alkane Waxes

Linear hydrocarbon chains, known as n-alkanes are among the most basic building blocks of organic matter, yet, very little is known about their structure and phase behavior at an interface. As major constituents of oils, fuels, polymers, and lubricants, they have also an immense industrial importance. The structure or organic and biological molecules like lipids, surfactants, and liquid crystals, which are formed from these linear chains, are of fundamental importance in understanding interfacial phenomena. New experiments, carried out by scientists from Brookhaven National Laboratory, Exxon, and BarIlon, Israel, demonstrate for the first time that the liquid/vapor interface induces an ordered surface phase at a temperature where the bulk remains disordered. This appears to be the simplest system in which surface-induced 2D crystalline ordering has been observed.

For most solids the surface melts before the bulk. Surprisingly, for n-alkanes, the free surface abruptly forms a hexagonally packed crystalline monolayer, where the long axis of the molecules is along the surface normal direction, at a temperature where the bulk remains an isotropic fluid. The surface normal structure has been deduced from modulated X-ray reflectivity profiles taken at the National Synchrotron Light Source, and the hexagonal in-plane structure has been determined from the symmetry of the X-ray diffraction pattern. This surface phase appears at about 3 degrees centigrade above the bulk solidification temperature. Motivated by the X-ray measurements, conventional surface tension measurements were carried out --versus the sample temperature. The abrupt and reversible change in the slope of the surface tension which occurs when the hexagonal surface layer forms, is easy to understand in terms of the relevant entropies as calculated from the bulk latent heat.

These studies have demonstrated that the surface of simple organic molecules becomes ordered at an interface where the bulk remains disordered. This is particularly significant since n-alkanes are the principal building blocks in many biological and chemical systems. The ability to correlate macroscopic properties (e.g., surface tension) with surface structure provides a thermodynamic basis for the observed interfacial phenomena. These measurements suggest the intriguing possibility that the latent heat of surface phase transitions can be extracted from surface tension measurements.

Oxygen-Isotope Exchange Occurs Slowly in Natural Systems

Partitioning of stable isotopes between minerals and solutions provides some of the key data used in estimating temperatures of initial crystallization and recrystallization in the natural environment. This is particularly important in sedimentary basins containing oil and gas, in geothermal systems, and in tracing the effects of fluid transport in geologic media. Knowledge of the time it takes to achieve isotopic equilibrium in model cases provides a better foundation for assessing the significance of estimated temperatures.

Recent experimental studies of the system $CaCO_3$-H_2O-NaCl by Dr. David Cole at Oak Ridge National Laboratory demonstrate that attainment of isotopic equilibrium in the exchange of ^{16}O and ^{18}O between calcite and coexisting fluid is a very slow process at temperatures and pressures corresponding to depths of less than 5 km in the Earth's crust. Rate constants were experimentally determined for experiments conducted at 300-600°C and extending from 8 to 81 days. Activation energies were calculated at 0.1gPa for water and 4m NaCl solutions coexisting with calcite. Data acquired as a function of pressure provided a basis for calculation of activation volume which is negative for both water and 4m NaCl. Rate data are then used to compute approximate time periods necessary to achieve the extent of isotopic exchange under specified conditions.

For example, using a closed system at 0.1gPa with a fluid/calcite mass ratio of 0.1 and an initial grain size of 0.025 cm, the time to attain oxygen isotope equilibrium is about 10 years at 500°C and 0.5m NaCl, and 3 years at 500°C and 4m NaCl. Extrapolation of the rate data to 200°C indicates an equilibration time of approximately $2.4X10^4$ years for H_2O and $1.5X10^4$ years for 4 m NaCl solutions for this case.

New Technique Facilitates the Study of Combustion Intermediates

Scientists at Harvard University and Brookhaven National Laboratory, with support from the Office of Basic Energy Sciences/Chemical Sciences Division, have developed and combined spectroscopic and molecular beam techniques to provide a new tool for identifying and characterizing combustion intermediates. Using supersonic jet flash pyrolysis, molecules are raised to high temperatures very rapidly, dissociated, and, before they can react, the intermediates are expanded into a vacuum where they can exist for periods of time long enough for study. Combining this source of transient combustion intermediates with a spectroscopic method known as Zero Kinetic Energy-Pulse Field Ionization, highly accurate ionization potentials of the intermediates can be measured and from these, chemical bond energies and other thermodynamic properties can be determined which may be used in computer models for combustion. The method has been tested on several species such as the methyl radical, CH_3, and will be applied to investigations on radical species containing three carbon atoms which are believed to be implicated in the formation of soot.

Molecular Dissociation Induced by Ion Collisions

Scientists at Kansas State University supported by the Office of Basic Energy Sciences/Division of Chemical Sciences have reported the first measurements showing that the angle formed by a molecule's internuclear axis and the ion projectile direction in a collision is an important factor in molecular dissociation, an effect first predicted by theory in 1960. The results are in agreement with quantum theory and will improve understanding of the dynamics of ion collisions found in gaseous plasmas. In the experiment, an accelerator-produced ion beam of fully stripped oxygen atoms was crossed with a collimated jet of hydrogen molecules. Each molecule transferred an electron to the colliding ion and immediately dissociated. Since the dissociation is much faster than the rotation of the molecule, the hydrogen atoms/ions flew apart after the electron transfer while the molecule was essentially frozen in position.

The maximum dissociation probability was found to occur when the molecular axis was perpendicular to the ion beam. In addition, an interference effect was observed and associated with scattering of the ion projectile from each of the two atoms in the molecule. The interference was found to be similar to that manifest in Young's two-slit experiment. The results are in agreement with quantum theory and will improve understanding of the dynamics of ion collisions found in gaseous plasmas.

Chaotic Particle Dispersion Process Better Understood for Plain Mixing Layers

Research carried out at Washington State University under the sponsorship of Office of Basic Energy Sciences/Engineering Research Program casts a new light on the way particles are dispersed in mixing layers. The resulting enhanced understanding of how dispersion takes place will aid in better design of particle feed jets in coal-fired power plants and of liquid droplet fueled combustion. It has been known that in free shear flows the dynamics is controlled by a large, nearly two-dimensional span-wise structure in which there is imbedded a somewhat smaller scale three-dimensional structure. It has now been found that an assembly of particles with sizes such that their aerodynamic response time is comparable with the time scale of the large scale spanwise structure undergoes a stretching and folding sequence. This process, apparently identical with that occurring in deterministic chaotic transformations, leads to spatial dispersion of the particles.

Vacancy Model Developed for Surface Diffusion on Semiconductors

A thorough, quantitative investigation of the surface diffusion of antimony on germanium has been completed using the newly-developed technique of Optical Second Harmonic Microscopy. These results may be explained semiquantitatively by a new model based on vacancy-mediated diffusion. The coverage dependence arises through an islanding mechanism in which immobile islands of antimony pin down the otherwise mobile germanium surface layer. The model predicts that the presence of a near-atmospheric pressure ambient should not significantly affect the diffusion parameters because they are dominated by the thermodynamics of vacancy formation. The first quantitative measurements of surface diffusion under such conditions (100 torr of helium or 5 torr of argon) have confirmed this prediction.

Reliable measurements of surface diffusion on semiconductors are practically nonexistent because most available methods either damage the surface or measure diffusion too indirectly to be reliable. However, surface diffusion is a critical step in the chemical mechanisms for thin-film deposition. Slow diffusion results in highly defected, poor-quality material. Particularly lacking are surface diffusion measurements at the temperatures characteristic of thin-film growth; most measurements are performed at much lower temperatures. This new method of second harmonic microscopy allows measurements of surface diffusion under processing temperatures and has shown that the fundamental mechanism for surface mobility can change under these conditions.

Furthermore, the model predicts that surface diffusion may be influenced by such process parameters as substrate carrier concentration and photon illumination. This suggests that additional control and enhancement may be possible during processing. This research is supported at the University of Illinois by the Office of Basic Energy Sciences/Division of Materials Sciences.

Determination of the Atomic Structure of Transition Metal Ions

The most stringent test involving the understanding of atomic structure is that involving hyperfine energy levels as it requires both measurements at the highest resolution in addition to calculations that describe the high-precision measurements. The spectroscopy of large atomic number ions, particularly those of the transition metals, is complicated by relativistic effects that originate in the strong interaction between the nucleus and its outer electrons. When the nuclear interaction is considered along with that amongst the electrons the theoretical questions expand to a many-body problem which is not amenable to solution by the popular independent particle theory.

Now a joint laboratory (Argonne National Laboratory) and university (Michigan Technological University) collaboration, with support from the Chemical Sciences Division, has made a substantial improvement in the experimental and theoretical understanding of the hyperfine structure of such heavy ions. The new high-precision measurements were made at Argonne National Laboratory using a high resolution laser-ion beam spectroscopic technique. The ab initio relativistic Configuration Interaction theory was developed at Michigan Technological University. The calculations demonstrate the capability of the new theoretical approach, which includes many body effects, to evaluate hyperfine structure with an accuracy at the 10% level in transition metals. The new approach will be extended to atoms with more electrons to ascertain the general nature of the solution.

Atomic Force Microscope Maps Atomic Topography and Friction

For the first time, atomic scale frictional force maps of a platinum stylus dragged over a gold (111) metal surface have been produced simultaneously with maps of the atomic corrugation of the gold surface.

Researchers under the direction of Dr. Miquel Salmeron at the Center for Advanced Materials have developed a unique bidirectional Atomic Force Microscope that is capable of applying a nanonewton compressive force between the very sharp tip and the surface - a force so small that single atomic bonds are not broken during the scan.

By simultaneously mapping surface topography and measuring the "dragging" or frictional force of the tip, the group was able to correlate the two and show that they have a similar atomic periodicity although the tip crossed directly over the centers of every third atom and therefore major peaks of the frictional force image are separated by three atomic bond lengths.

Similar studies using tips and surfaces to which defined compounds have been adsorbed are being carried out to explore the mechanisms underlying lubrication, adhesion and the interaction between surfaces.

Wave Dynamics Modeled for Falling Liquid Film Surfaces

Falling liquid films play a major role in many processes, e.g. optical fiber coating, paper coating, scrubbing of industrial gas effluents, and heat exchangers. Evolution of waves on the film surfaces adversely affects the uniformity of coatings, while enhancing heat and mass transfer rates. Experiments have shown that the initial exponential growth of a surface instability leads to the formation of "solitary" waves propagating at a constant speed while retaining their shape. Eventually, as spanwise instabilities set in, the waves break up, and the orderly structure become turbulent.

Work carried out by Professor H.-C. Chang (Notre Dame) has provided a theoretical description of the propagation of the solitary waves on falling films prior to disruption. It is in excellent agreement with the observations. The enhanced understanding of the mechanisms underlying the propagation and disruption of the waves on falling liquid film surfaces will contribute to controlling their adverse effects, while exploiting the beneficial ones.

Planar Structure Found for an Important Combustion Intermediate

Nearly four years ago scientists at Argonne National Laboratory reported the first observation of an important combustion intermediate, COOH, in the gas phase. This intermediate exists momentarily in the reaction of OH with CO to give H atoms and CO_2 which is the final step in the oxidation of carbon-based fuels. The continuing study of COOH has been taken up by scientists supported by the Chemical Sciences Division, of the Office of Basic Energy Sciences at Brookhaven National Laboratory and the State University of New York at Stonybrook. In collaboration with colleagues at the Harvard Smithsonian Center for Astrophysics, they have reported recently in the Journal of Chemical Physics the rotational spectrum of COOH from which they have deduced its structure. The structure is that of planar HOCO in its trans (zigzag) form. Some of their observations suggest that it may also exist in a cis (flattened W shape) form. The significance of this work is related to the stability of both species and the effects their stabilities have on the speed of the chemical reaction. This work has brought us one step further in our ability to understand and model combustion reactions. It also exemplifies the benefits of close interactions among scientists of different backgrounds in addressing such complex processes as combustion.

Grain Boundaries in Metals Have 20-30% Missing Atoms

Computer simulations by Dr. S. R. Philpot of Argonne National Laboratory have shown that grain boundaries in elemental metals are zones of significant reconstruction in which 20-30% of the atoms are missing from the atomic planes adjacent to the boundary. This result is in contrast to the common assumption that the crystal structures of the two adjacent crystals are continuous up to the boundary and, with the exception of misfit locations at the boundary, that little or no reconstruction occurs. Philpot's work shows that the boundaries achieve a minimum energy when reconstruction occurs with removal of atoms in the grain boundary zone. The computer simulations also show that the reconstruction significantly affects the elastic properties of the grain boundaries. These results suggest that other properties such as adsorption of impurities, catalytic effects and electrical properties may be affected by the occurrence of grain boundary reconstruction. This study was funded through the Office of Basic Energy Sciences/Division of Materials Sciences.

Neutron Scattering Measurements of $YBa_2Cu_3O_7$ Provide Important Insights

Vortices play a crucial role in the current-carrying capability of superconductors. Now, scientists at the Oak Ridge National Laboratory, have successfully measured the vortex lattice in $YBa_2Cu_3O_7$, one of the most important of the cuprate, high-temperature superconductors, using small-angle neutron scattering techniques. The technique utilizes the fact that neutrons have a magnetic moment that interacts with the field distribution inside the superconductor. The results showed a square vortex lattice pattern for a field parallel to the crystal c-axis, rather than a triangular lattice, which is usually the lowest energy state. The square pattern is found because of the strong pinning caused by the twin boundaries when they are parallel to the vortex line. The strong pinning provided by the twin boundaries demonstrates that the best pinning centers are those that extend along the length of the vortex line. This is very important in designing pinning centers to provide high critical currents.

Reverse Micelles Behavior Better Understood for Supercritical Fluids

Research on supercritical fluid/reverse micelle systems has led to the first evidence for external pressure altering the structure of water about a solute in the core of reverse micelles. This work suggests that the bulk solvent density of near-critical propane can influence the rate of water structural reorientation within the interior of the reverse micelle. This then opens opportunities for unique applications in separations, extraction, enzyme catalysis, and other chemical reaction processes. A reverse micelle is a self-assembled macromolecular structure consisting of surfactant molecules surrounding a central water core that is isolated from the bulk supercritical solvent by the surfactant molecules. This novel investigation of the pressure-assisted control of the water core solvent relaxation rate will further the basic understanding of the solution dynamics between the micelle and the fluid and between the fluid with the water core. The reported micelle observations were made by Frank Bright at SUNY-Buffalo with support from the BES/Chemical Sciences Division.

Observed Spectrum of Visible Radiation Altered for Multi-Atom Systems

Research carried out by Professor E. Wolf (U. of Rochester) on the propagation of partially coherent radiation has revealed observable spectral effects in multi-atom systems due to their interaction with their own electromagnetic field. That is analogous to such one-atom/radiation field interaction as those leading to natural decay lifetime, and to the Lamb shift. Specifically, radiation interaction between a pair of atoms changes the lifetimes and resonance frequencies of the relevant atomic transitions. Moreover, spectra of emitted radiation are changed by the correlation between the fluctuation of the atomic polarizations. These results contribute to better understanding of radiative transfer processes, and, as pointed out by a reviewer of the recent grant renewal application from Professor Wolf, of emission from synchrotron light sources. This research was carried out under BES/Engineering Program support.

Prediction of Useful Safe Lifetime of Irradiated Nuclear Reactor Components

It has been shown that gamma-rays generated from neutron capture reactions are considerably more important than previously suspected in producing freely migrating defects which in turn cause lifetime limiting property changes in reactor components. It had been known for almost two decades that the efficiency for producing freely-migrating defects decreased with increasing neutron recoil energy. However, it was only in the past few years that it became possible to demonstrate how unexpectedly large this decrease actually was. Recent results showed that less than one per cent of the number of defects given by standard displacements per atom (dpa) algorithms become freely-migrating as a consequence of energetic atomic displacements typical of fast neutron irradiations. It is well documented, however, that void swelling in reactors involves more than one per cent of the calculated number of defects. This recent finding indicates that mechanisms other than energetic displacement cascades must be generating freely-migrating defects during neutron irradiation. Now, calculations have been performed showing that Compton electron production by neutron-capture gamma-rays apparently provides an additional source of freely-migrating defects in reactor environments.

This new finding that gamma-rays could generate substantial numbers of freely migrating defects in neutron irradiation environments may have significant bearing on the ability to predict accumulated radiation induced property changes resulting from defect-coupled mass transport in reactor materials. In particular, this finding could provide a new basis for correlating property changes in different neutron test facilities and for predicting the useful lifetime of critical reactor components, rather than waiting for dangerous failure to occur. This work was carried out by Drs. L. E. Rehn and R. C. Birtcher, Materials Science Division, Argonne National Laboratory.

Laser Fluorescence Analysis Reveals Microscopic Defects in Surfaces

Basic research on the interaction of laser light with inorganic crystal surfaces has led to the discovery of a laser fluorescence technique possibly applicable to the microscopic characterization of the materials exterior. It was noted that dislocations or vacancies in the orderly array of atoms on the surface of an inorganic crystal are observable by their blue fluorescence under low intensity ultraviolet laser irradiation. Investigators now have an optical method for identifying surface defects and removing them before they propagate and weaken the material. It was also discovered that laser ablation of surfaces occurs along these blue fluorescing cracks. This new fluorescence technique can be used to further understand and control the laser ablation process at the micron level for the fabrication of tougher ceramics or more nearly perfect optical materials. This discovery by Chemical Sciences investigator Tom Dickinson at Washington State University was featured in the December 12, 1992, issue of *Science News* in "Science News of the Week."

Researchers Map Residual Stresses in Multipass Welds

The application of neutron residual stress measurement technology has been expanded to include mapping of stresses formed as a result of complex, multipass welds. A multipass weld is often used to join thick plates such as those used in nuclear reactor and steam pressure vessels. Quantitative knowledge of the stress state after welding is critical to predicting structural integrity and therefore the safety of pressure vessels and other highly loaded structural components. The complexity of the multipass welding process makes prediction of the resulting stress state extremely difficult. Until now, often the only effective way to compensate for such hard-to-quantify residual stresses was through trial and error testing in product development. Thermal neutrons from the High Flux Isotope Reactor (HFIR) were used to perform the first nondestructive 3D mapping of residual stresses within a plate containing a multipass weld. The stress mapping of a ferritic steel plate joined with a multipass weld revealed that the maximum residual tensile stress level was buried within the weld metal and is oriented along the weld bead. This maximum stress was 50 percent higher than the residual stress near the surface. This important information can only be obtained with neutron diffraction techniques. This data will assist in the development of models to predict the resulting stress state in welding applications.

Additional neutron residual stress mappings have been performed on a number of systems including ceramic engine components (e.g., thermal barrier coatings on pistons provided by Cummins Engine) and vibratory stress relief processes for welding improvement (with Concurrent Technologies). These demonstration projects show the broad range of the technique and the potential of quantitative, nondestructive stress analysis.

The research was performed by Drs. C. R. Hubbard, S. David, and S. Spooner of Oak Ridge National Laboratory (ORNL), and J. Root and T. Holden of Chalk River Reactor, Canada. It was jointly sponsored by the BES/Division of Materials Sciences and the ORNL Laboratory Directed Research and Development Program.

Chemical Vapor Deposition (CVD) Better Understood Through Disilane Deposition

The initial chemisorption, dissociation, and pyrolytic reactions of individual disilane (Si_2H_6) molecules on the surface of a germanium crystal have been examined as a means of characterizing the CVD mechanism for epitaxial growth of silicon on germanium. The evolution of the chemical states was observed through the formation and decomposition of various hydride species on the surface, e.g., SiH_3, SiH_2, SiH and GeH. Also observed were the formation of clusters and islands on the surface, island coarsening, step flow, intermixing and in-diffusion of silicon, and the multilayer growth of silicon via atomic layer epitaxy. This is a prototypical system; the detailed, step-by-step description is fundamental to the understanding of CVD as an industrial approach to epitaxial and thin film formation and processing for numerous electronic and other applications. The research was performed by Professor T-C. Chiang, University of Illinois Materials Research Laboratory, as a part of a BES/ Division of Materials Sciences Program.

Time-Resolved X-ray Scattering Studies Show Layer-by-Layer Epitaxial Growth

Scientists from AT&T Bell Laboratories, IBM Watson Laboratory, and the Stanford Synchrotron Radiation Laboratory (SSRL) have observed the layer-by-layer epitaxial growth of Gallium Arsenide (GaAs) using X-ray diffraction techniques and the very bright X-ray beams made possible from the 15-period wiggler at SSRL. During the vapor-phase epitaxial growth of crystals, a variety of growth modes occur, including a rough three-dimensional mode at low temperatures which changes to layer-by-layer growth at higher temperatures. At even higher temperatures, step-flow growth eventually dominates. The presence of layer-by-layer growth in electrochemical deposition has been inferred for 20 years (generally through the use of interrupted high energy electron diffraction studies), but has not been observed in-situ because of high ambient pressures and/or the presence of magnetic fields which preclude the use of electron diffraction techniques.

Oscillations in the intensity of the (1,1,0.05) diffraction peak were observed as a function of time following the introduction of tertiarybutylarsine and trimethyl gallium into the growth chamber. The period of the oscillations is of the order of 1 second for each bilayer. Further analysis of the diffracted X-rays yields the size and shape distributions of islands formed during the growth process. It also appears that these islands are not randomly nucleated but have positions which are correlated. This new technique will provide insight into the growth mechanisms of the chemical vapor deposition process, and could lead to improved interfaces which are important for optimum performance of semiconductors and solid state optical devices. These results were published in the November 9, 1992, issue of *Physical Review Letters*.

Isotopic Dating Methods Show Two Sudden Climate Changes

Micheal T. Murrell of Los Alamos National Laboratory has developed new methodology for high-precision mass spectrometric uranium-thorium-series dating. It results in improved resolution of U-, Th-series dating of the last 500,000 years from $\pm$10% to $\pm$<1%. This accomplishment permits high-resolution examination of the global climate change record necessary to distinguish smooth climatic transitions from step alterations. A report in *Science* (December 4, 1992) illustrates how the new method is combined with stable carbon and oxygen isotopic measurements of carbonate samples from Cold Water Cave in northeast Iowa. These integrated data are used to define midcontinental climatic changes 1,000-10,000 years ago. Significant shifts in the stable isotopic record coincide with well-documented vegetation changes and suggest that temperatures increased by about 3° at 5,900$\pm$42 years and then cooled again by 4° about 3,600 years ago. Initiation of the carbon isotope increase at 5,900 years suggests that an equilibrium prairie vegetation was not attained until significantly after 3,600 years. The results suggest that Pacific air masses reached midcontinent by 5,900 years and were replaced by Arctic air at around 3,600 years. These results can be incorporated into the feedback mechanisms and atmospheric linkages needed to provide historical data used in modeling global climate change. Support for this research is provided through the BES/Geosciences Research Program.

Model Simulates Complex Sheet Metal Forming Problem

The polycrystalline metal plastic deformation model developed at Los Alamos National Laboratory (LANL) under the BES/Materials Sciences program has now been incorporated into a finite-element code (developed under Office of Naval Research (ONR) funding) and was used to simulate the deep drawing of an aluminum cup. Plastic deformation is characterized by a non-linear stress-strain relationship, irreversible behavior, and directional anisotropy. The anisotropy of plastic deformation can have severe influences on metal forming operations. By far the most important cause of plastic anisotropy is due to textures in the starting materials and texture development during the process. Texture development is a phenomenon that can only be quantitatively described by polycrystal simulation. This work demonstrates that future problems involving plasticity and severe anisotropy can be realistically solved on the basis of fundamental understanding by using finite-element codes with embedded materials behavior codes such as the polycrystal model. The collaborants involved in this work are A. J. Beaudoin and P. R. Dawson (both ONR-funded from Cornell University), K. K. Mathur (from Thinking Machines Corporation), and U. F. Kocks (from LANL).

Standard Reaction Rate Theory Does Not Hold for Important Combustion Reaction

For nearly 40 years RRKM theory has been the most important theoretical tool for predicting and extrapolating the rates of chemical reactions. The theory is named for the initials of the last names of its developers, the last of whom, Professor Rudolph Marcus, won this year's Nobel Prize in Chemistry. The first experimental observation of one of the theory's principal features—the dependence of the rate on the vibrational energies of a transition state between reactants and products—was recently reported.

Following closely on that experimental tour de force, comes another study on the most fundamental and important reaction in the chemistry of combustion: $H+O_2 \rightleftharpoons OH+O$. Scientists at the Combustion Research Facility (CRF) at Sandia National Laboratories, Livermore, have demonstrated that this reaction shows pronounced non-RRKM behavior. RRKM theory predicted a rate for this reaction that was twice as fast as experimentally observed in the temperature range from 200 K to 5000 K. Using a more exact quasi-classical trajectory calculation, rate coefficients were found to be in excellent agreement with experiment, demonstrating that the error was in the RRKM theory and not the experimental measurements.

The basis for RRKM theory is the statistical distribution of energy in the vibrational motions of a transition state complex. For systems consisting of few atoms, the statistical averaging is not possible because of the limited number of vibrational motions among the atoms. The CRF calculation showed that collisions between OH and O preferentially returned to OH and O and collisions between H and O_2 preferentially returned to H and O_2. The RRKM breakdown is due to the mismatch between the O-O and the O-H vibrational motions in the transition state complex. Research will continue on determining the circumstances under which RRKM theory can be used reliably.

Powerful New Research Tool for Atomic Physics Introduced

In solving a 50-year-old problem, an international team, involving ORNL scientists supported by the BES/Division of Chemical Sciences, has demonstrated the usefulness of an ion storage ring with electron cooling technology. Using the new facility at Stockholm, CRYRING, the team of 11 scientists measured the rate coefficient for the dissociative recombination of the singly charged hydrogen triatomic ion, H_3^+, i.e., H_3+e H+H+H or H_2+H. This reaction is important to the understanding of stellar evolution since it is the precursor to the formation of over 100 molecules involving the protonation of oxygen, carbon, and other atoms.

In the definitive experiment, the ions were circulated in the storage ring for 8 seconds at 33 Mev. During each revolution the ions passed through a merged electron mean. By careful manipulation of the relative velocities of the merged ions and electrons, the ions collided with the merged electrons and were cooled by transferring kinetic energy to the electrons. Only at specific relative velocities, ideally at zero, do the electrons combine with the ions to yield the products that are the unequivocal signature for recombination.

Earlier measured rates of this important process using other techniques were in great disagreement. The rates reported ranged over four orders of magnitude. It was eventually recognized that the measured rate was strongly dependent upon the vibrational state population of the initial H_3^+ ion. The inability to control this parameter in the earlier experiments was found to be the source of disagreement. The new ring stored the ions sufficiently long to assure cooling to the ground vibrational state. Data was obtained over four orders of magnitude, between 0.0025 and 30 ev, with excellent signal-to-noise. Future experiments using this new technology are expected to continue yielding new and exciting results.

Diagnostic Technique Beneficial for Materials Processing Using Plasmas

Researchers supported by the BES/Engineering Research Program at Stanford University have reported the successful use of a sophisticated optical method, the so-called degenerate four wave mixing technique, to monitor nonequilibrium concentrations of certain important species in plasmas used for materials processing.

The fast deposition of hard diamond coatings on soft metallic substrates can be carried out at near-atmospheric pressures, provided that the appropriate nonequilibrium plasma composition is maintained. Normally at such pressures, equilibrium conditions prevail and special measures need to be taken to maintain the necessary state of the plasma. The ability to do that depends critically on the ability to measure that state. Degenerate four-wave mixing has now been shown to be an effective tool for that purpose. This capability should be important for understanding and control of plasma chemistry kinetics and, hence, lead to novel approaches to materials synthesis and processing.

Major Contribution to Catalytic Chemical Dynamics Reported

Understanding the nature and energetics of intermediate species is key to the technological exploitation of the potential inherent in controlling bond-selective chemistry. A unique and important feature of catalysis research is the study of chemical dynamics of photoinduced atomic and molecular processes on metal and semiconductor surfaces. Prominent examples of catalytic reactions are those initiated by a change in the equilibrium configuration of the absorbed species through the addition or removal of an electron by photon stimulated desorption. A major step has been taken by NIST scientists in understanding these processes by documenting the photodesorption of nitric oxide (NO) on platinum metal surfaces, a research effort supported by the Division of Chemical Sciences. They found that photons impinging on an NO-covered surface produces a flux of electrons (photoelectrons) from within the substrate that impinge upon the adsorbed NO molecules. This results in the formation of a transient negative molecular ion. After a short time, in the order of a few femtoseconds, the electron leaves the ion and returns to the surface but before it does, some of the energy that accompanied the electron initially is distributed to chemical bonds of the adsorbed molecule as vibrational and rotational energy, providing sufficient internal energy to allow desorption of the molecule. This understanding, now embodied as a theory of hot electron mediated laser desorption involving the resonant capture of photogenerated carriers by the absorbate, is a major contribution to the area of catalytic science.

Research Opportunities Identified in Plant Biochemistry

The Energy Biosciences program sponsored a workshop designed to outline the status of plant biochemistry and the opportunities for major applications of the knowledge. The workshop was held in Kona, Hawaii, on December 11-13, 1992, with 29 participants affiliated with universities, industry, and government laboratories. Extensive discussions were held on the research needs and opportunities that would advance the knowledge of the capabilities of plants to metabolize substrates and how such information will benefit society in the future. A summary of the workshop was drawn up by the workshop organizer, Dr. Chris Somerville of Michigan State University. The report was published after careful editing of a draft by the participants and also many other experts who were not workshop attendees. Copies of the report are available from the Energy Biosciences Division (301-903-2873).

Theoretical Advances Reported on Semiconductor Clusters

New theoretical methods have been developed for calculation of the size dependence of bandgap energies for colloidal semiconductor particles in the BES/Chemical Sciences-supported research carried out under the direction of Professor Richard Friesner at Columbia University. The calculated optical excitation energies for CdS particles are in excellent agreement with bandgap energies measured experimentally at DuPont. For GaP, GaS, and Si clusters, the computer simulations have furnished predictions of the heretofore unknown optical excitation spectra and energy levels of the particulate semiconductors. The theory predicts, for the latter, a shift in the bandgap to the blue followed by a reverse shift to the red in the absorption spectrum as the size decreases, when compared with the bulk semiconductor. In continuing studies, quantum chemical refinements to the model for the molecular surface of the cluster should allow for calculations of electron trapping, electron-hole recombination, and electron transfer kinetics at the semiconductor/liquid interface.

Random Cracking of Solids Does not Affect Elastic Properties

Studies supported by BES-Engineering Research Program at Tufts University (M. Kachanov) have revealed an important property of solids with randomly distributed cracks. Specifically, it was found that the effective elastic properties of such solids are adequately described by neglecting the interactions between the cracks. It so happens that for randomly located cracks, the two primary sources of crack-to-crack interactions, namely stress shielding and stress amplification, cancel out. Hence, to a good approximation, the cracks may be treated as if they were not interacting at all. This finding should considerably reduce the computational effort in many safety-related engineering calculations.

Control of Metallic Impurities in Silicon Through Trapping Microscopic Cavities

Dr. Sam M. Myers of Sandia National Laboratories/Albuquerque, with support from BES/Division of Materials Sciences, has discovered that microscopic cavities within silicon provide exceptionally effective traps for metallic impurities. Transition metal impurities, even at very low levels, are known to degrade the performance of silicon-based microelectronics. Thus, this finding potentially provides an important new approach for the technology of "gettering," in which impurity traps in sacrificial regions of silicon wafers are used to remove detrimental metallic impurities from active device regions.

Dr. Myers formed cavities within silicon by ion implantation of helium and subsequent heating, which produced bubbles in the nanometer size range followed by helium diffusion out of the material. The trapping effect was investigated for a representative impurity, copper. This species was introduced by ion implantation, and its movements to and from the cavity-containing region of the silicon during heating were observed by ion-backscattering analysis. It is particularly significant that the cavities were observed to trap copper more strongly than silicon lattice defects, which have previously been used for impurity gettering. The exceptionally effective binding is proposed to occur at the internal surfaces of the cavities, where highly reactive silicon dangling bonds protrude into an unobstructed void.

From the standpoint of impurity gettering in silicon technology, the above microscopic cavities appear attractive because 1) their creation is convenient and well controlled, 2) they are structurally stable to high temperatures, 3) the binding of impurities is exceptionally strong, and 4) relatively large numbers of impurities can be accommodated (10^{16} copper atoms per square centimeter of wafer surface demonstrated).

<u>Novel Ion Imaging Technique Improves Analyses of Biological Samples</u>

Basic research by BES/Division of Chemical Sciences investigators at ORNL has lead to the development of a new analytical technique in mass spectroscopy for the ion imaging of biological tissue samples. This technique uses a primary ion beam to interrogate the surface of the tissue sample. Secondary ions are produced from the sample surface whose mass is indicative of a drug or its metabolites. These secondary ions are then mass analyzed and their distribution determined with the imaging capabilities of the instrument. This capability results from a specially designed organic secondary ion microprobe/mass spectrometer and could prove important in pharmacology and toxicology studies of biological specimens. The combination permits acquisition of data necessary to determine the distribution of targeted organic analytes even in the presence of extreme isobaric interference. With this system, large samples (1 cm. in diameter) can be viewed in their entirety, and distributions of very dilute analytes can be produced. These features are important in the analysis of biological tissue samples and reflect sizes comparable to those currently analyzed by autoradiography. This novel ion imaging technique is more rapid than contemporary methods for obtaining spatial distribution and identifying drugs and their metabolites in tissue samples. This technique has significant implications in the continued monitoring of potential adverse health effects of human exposure to radiation and energy-related processes.

<u>Unsymmetrically Labeled Oxygen Molecules Used to Elucidate Oxygen Metabolism</u>

A new method for producing large quantities of unsymmetrically labeled oxygen molecules has been discovered through chemistry research at Argonne National Laboratory in collaboration with researchers at Tel Aviv University in Israel. Earlier studies with the unsymmetrical oxygen molecule produced by way of the reaction of oxygen-18 labeled hypofluorous acid, HOF, with water resulted in elucidating the iron-oxygen bonding in hemoglobin. The discovery that HOF is quite stable in acetonitrile has now provided the ability to produce the $^{16}O^{18}O$ molecule in large quantities and has made it possible to do an experimental study which has led to the understanding of the reduction of molecular oxygen by the enzyme cytochrome oxidase, a key step in the course of biological metabolism. This was done in collaboration with researchers at the Institute for Molecular Science at Okazaki, Japan and at Michigan State University. Results show that a Raman band previously assigned to iron(III)-peroxyspecies actually belonged to a subsequently formed iron(IV) species, which altered the representation of the oxygen interaction sequence. This Chemical Sciences supported work has been accepted for publication in the *<u>Proceedings of the National Academy of Sciences</u>*.

Assemblies of $Al_{12}Si$ Clusters Form Novel Super Crystal

A scheme to produce super crystals, or crystals assembled from clusters as opposed to the conventional practice of assembling from atoms, was reported in a recent issue of *Physical Review Letters* (September 14, 1992) and also featured in the September 17, 1992, issue of the *Science News* in "Science News of the Week." Materials Science grantees S. N. Khanna and P. Jena of Virginia Commonwealth University demonstrated that by selectively altering the number and type of atoms it is possible to construct clusters that are not only stable energetically, but can also be stable against reactions. Such clusters can then be assembled to produce crystals with unusual electronic and optical properties. Using state-of-the-art quantum mechanical codes, they have demonstrated that $Al_{12}Si$ is one such cluster. This cluster has closed electronic shells with forty valence electrons and is 7.7eV lower in energy than an Al_{13} cluster. the bottom line: whereas 8 percent Si in Al would likely be a normal metallic alloy, a crystal made from clusters with the same composition is predicted to be an insulator. Therefore, this super crystal will have uncommon electronic and optical properties.

Geothermal Systems Found to be Dependent on Climate

Evidence of past geothermal activity within the inner trough of the northern Kenya Rift Valley includes eroded hot-spring siliceous sinter and silica vein deposits on the upper flanks and summit areas of several young volcanic centers. Uranium-series ages for these hydrothermal silica deposits indicate that times of enhanced geothermal activity correlate with times of high paleolake levels (i.e., humid climatic periods). Thus, geothermal activity in the rift is modulated by climate; elevated water tables and increases in the availability of rainwater for deep convective circulation promote transfer of heat and mass to the surface from deep and long-lived heat sources. These findings indicate that rainfall and climatic change must be considered explicitly in addition to the aquifer recharge term used in conventional geothermal reservoir analysis.

These conclusions were drawn using Uranium series ages, based on $^{234}U/^{238}U$, $^{230}Th/^{232}Th$, and $^{230}Th/^{234}U$ isotopic ratios, by Argonne National Laboratory geochemist Neil Sturchio, in collaboration with scientists from the British Geological Survey. These findings have been submitted for publication in *Nature*.

Anomalous Interplanar Expansion at Beryllium Surface

For more than a decade, the Office of Basic Energy Sciences (BES)/ Materials Sciences program at Oak Ridge National Laboratory (ORNL) has had one of the world's most successful programs in using low-energy electron diffraction (LEED) for the determination of atomic structures at surfaces. For example, early work at Oak Ridge National Laboratory showed that the Cu(110) surface has a large (about 10%) contraction of the first interplanar spacing, which is the distance between the first and second atomic layers of the surface. Results of subsequent investigations at ORNL and elsewhere for various surfaces have lead to an almost universal rule that the first interplanar spacing is contracted from the bulk value while the second spacing is expanded.

Concurrently, others have formulated theories to provide explanations for that experimentally extracted universal rule, with special concern being to provide reasons for the interplanar contraction. However, recent LEED work at ORNL has demonstrated the existence of a gross violation of the universal rule, since the work has shown that the Be(0001) surface has an anomalously large interplanar expansion of about 6%. Since valid reasons exist which indicate that this experimentally determined expansion can be in error by no more that 0.4%, and essentially all theoretical work to date would predict an interplanar contraction, the Be(0001) result provides an important new result to test developing theoretical models for surface atomic structure.

This new Be(0001) result has considerable significance because theoretical models for surface structure are only a subcase of general theories of pair potentials between atoms (or ions) in various nonbulk environments. Accurate pair potentials are required in any attempt to simulate materials and their properties by numerical means such as molecular dynamics. This research was performed by H. L. Davis of ORNL, and J. B. Hannon, K. B. Ray, and E. W. Plummer of the University of Pennsylvania.

Oxygen Ordering Influences Superconducting Transition

Computer simulation has provided considerable insight into the relationship between the oxygen ordering and superconducting properties in $YBa_2Cu_3O_x$ (YBCO). The model adopted in the simulation by a collaboration of G. Ceder (MIT), R. McCormack (Univ. of CA/Berkeley), and D. de Fontaine (LBL) was the "Asymmetric Next Nearest Neighbor Ising (ASYNNNI) Model," which very successfully describes ordered superstructure phase equilibria in YBCO. The notion that the superconducting transition temperature T_c could be influenced by oxygen order, already anticipated in this theoretical work, received spectacular confirmation from the experimental studies of B. Veal, J. Jorgensen and co-workers at the Argonne National Laboratory. The Argonne group found that far off-stoichiometric samples of $YBa_2Cu_3O_x$ ($x = 6.45$) quenched rapidly to room temperature exhibited an increase in T_c by as much as 20 degrees during aging. It was concluded that only oxygen rearrangement could be responsible for this remarkable temperature rise.

The ASYNNNI model clearly indicates that thermodynamic equilibrium favors the formation of long O-Cu-O chains in YBCO, regardless of oxygen stoichiometry. Fragmented chains produce incorrectly O-coordinated Cu atoms in the "chain" plane, thereby raising the total bonding energy. The progressive elimination of chain ends increases the concentration of electron holes in YBCO, thereby tending to increase T_c. The rise in the frequency of correctly coordinated (2-fold and 4-fold) Cu sites and the concomitant decrease in that of incorrectly coordinated (3-fold) sites on the one hand, and the rise in T_c as observed by the Argonne group on the other hand evolve similarly as a function of time. The experimentally determined oxygen-concentration dependence of the effect is also matched closely by the simulation results. Thus, the appropriate O-coordination of Cu is responsible for optimal doping in the YBCO superconductor.

Diamond Monochromators Look Promising for Third Generation Synchrotron Light Sources

Scientists at Brookhaven National Laboratory, in collaboration with Professor Michael Hart of the University of Manchester (England), have achieved a technical breakthrough in the development of optical elements which can handle the extremely high power photon beams from advanced light sources. In many X-ray experiments, silicon single crystals are used to select monochromatic X-ray beams from a broad band of X-ray wavelengths. Achievement of such monochromatic X-ray beams is important for the study of the fine details of crystalline and magnetic structure in solids, the thermal motion of atoms in a crystal, and many other features such as the detailed electronic structure in solids. Third generation light sources such as the Advanced Light Source at Berkeley, and the Advanced Photon Source at Argonne, will generate extremely bright X-ray beams (beams of great intensity in a very narrow cone) which will allow many unprecedented experiments to be done because of the high brightness of photon beams incident on a very small area of a sample. However, in the monochromatization of a very high power X-ray beam, many of the photons are absorbed by the monochromator crystal, which heats the crystal causing it to expand locally, and this distorts (very slightly, but significantly) the narrow X-ray beam, thus loosing much of the high brightness.

The breakthrough comes about through the possibility of using single crystal diamonds instead of silicon to monchromatize a high power X-ray beam at the National Synchrotron Light Source. Comparison of the diffracted X-ray beams by crystals of silicon and by diamond show a large distortion of the X-ray beam by heating of the silicon crystal under a high power X-ray beam, but the high power beam is undistorted by the diamond. Diamond has a thermal conductivity of nearly 15 times that of silicon, and its thermal expansion is about half that of silicon, but maintains the same X-ray scattering power as silicon. In recent years, it has been shown that diamond films can be grown on many surfaces, and it is likely that optical elements can be made in this way for future monochromators to handle the extremely high heat loads from X-ray beams of third generation of light sources. Furthermore, when diamond is made from isotopically pure carbon, its thermal conductivity rises by another fifty per cent, which would further ensure the ability to provide a monochromatized, undistorted, high power X-ray beam to experiments.

Light-Assisted Synthesis of High-Value Chemicals Explored

Photooxidation by red and near-infrared light has potential as an inexpensive method for industrial chemical synthesis. The light of these long wavelengths is the most abundant form of energy from the sun, and it is the least expensive to produce artificially. In matrix-isolation spectroscopic studies at Lawrence Berkeley Laboratory, new reaction pathways have been discovered in formation of industrial chemicals by photooxidation of a variety of abundant, unsaturated hydrocarbons, using red and near-infrared light. The reactions between hydrocarbon and oxygen donor are studied in a specially designed, low temperature apparatus where they are loaded onto an inert, solid matrix. A key feature of the research is the use of tunable dye lasers for reactant excitation. The reaction mechanisms and dynamics of the resulting chemistry are monitored by trapping the chemical intermediates in the cryogenic solid environment and their structures determined by Fourier-transform infrared spectroscopy.

Converting Sound to Light

The phenomenon called "sonoluminescence," in which tiny gas-filled bubbles created by ultrasound collapse rapidly while emitting visible light, was first observed 58 years ago by German scientists who considered it but a curiosity. The phenomenon retained this status until this year, when Dr. Seth Putterman of the University of California at Los Angeles embarked on a Basic Energy Sciences/Advanced Energy Projects-supported study of its origins and characteristics to identify conditions under which light emission might be enhanced. He published his initial findings in *Physical Review Letters* 69, 1182, on August 24, 1992, reporting clock-like emission of picosecond pulses of light with peak power over 30 mW, originating from bubbles trapped at the velocity node of a resonant sound field in water. The light spectrum is reported to be broad band, unexpectedly extending into the ultraviolet. Future studies will include doping the bubbles with lasing dyes, and employing liquids that are more transparent to ultraviolet radiation.

Growth of Oxide Films on Metals

The Brookhaven National Laboratory (BNL) Corrosion Group under the direction of Dr. H. S. Isaacs, with support from the Basic Energy Sciences/Materials Sciences Program, has conducted an in-situ determination of the chemical changes taking place in very thin passivating oxide films that protect aluminum and iron alloys from corrosion in wet environments. The passivating oxide film is only about ten atom layers thick and its chemistry depends on the chemistry of the environment and any oxidizing voltage applied to the metal. Previously, high resolution studies of corrosion films have required the use of electron beams under high vacuum conditions. Such studies risked possible modification of the films in their removal from the wet environment. The use of penetrating x-ray radiation has allowed chemical changes in the film to be observed by x-ray absorption while the metal is in contact with a aluminum-chromium and iron-chromium alloys was found to depend on the applied oxidizing voltage. Under moderate oxidizing conditions, an insoluble form of chromium is formed, whereas under high oxidizing conditions a soluble form, chromate, is formed. This soluble form can be trapped in the oxide film and reversibly changed to the insoluble form by changing the applied oxidizing voltage in the cell. However, in aluminum-chromium alloys, if the voltage is increased too slowly, then the soluble chromate simply dissolves and is lost from the film so that the metal can then corrode. The soluble chromate trapped in the film on iron-chromate alloys is unstable in air and spontaneously reverts to the insoluble form over a few hours. The corrosion resistance of metals depend on the presence and behavior of the oxide layer that forms on the surface. This study has provided chemical insights into the mechanism of film formation and its environment and time-dependence.

Characterization of Paraffin Activation by a Metal Surface

In heterogeneous catalysis, a complete understanding of the initial activation of molecules on surfaces has been illusive. With paraffins, this activated surface species has lost a hydrogen atom and the alkyl fragment is chemically bound to the surface. Professor W. Henry Weinberg from the University of California at Santa Barbara has completed the first comprehensive characterization of the energetics and kinetics for propane and iso-butane activation on a corrugated platinum surface [Pt(110)-(1x2)]. The results include the true activation energies and preexponential terms which describe hydrogen abstraction from methyl (CH_3), methylene (CH_2) and methyne (CH) groups. The knowledge and methodologies developed here provide a clear and more complete understanding of the fundamental rate determining step in most surface reactions of paraffins. This work provides a first-step in understanding a fundamental link to making fuels and chemicals from low molecular weight paraffins.

Oxidation State Determined at a Buried Interface

Several surface-sensitive techniques are available for the characterization of oxidation state, including Auger electron spectroscopy, x-ray photoelectron spectroscopy, and electron energy loss spectroscopy. Oak Ridge National Laboratory (ORNL) scientists have developed the first technique that is sensitive to the oxidation state at a buried interface. This technique has many potential applications. Atomic absorption edges are experimentally accessible for all elements above calcium in the periodic table; for lighter elements, x-rays are a surface-sensitive rather than a penetrating probe for most materials. Interface diffraction can be measured for interfaces between single crystals and films which are crystalline, amorphous, or even liquid. In future applications, the effects of interface chemistry on the epitaxy, electronic, and mechanical properties of interfaces will be explored. The research has been supported by the Division of Materials Sciences.

The cross sections of an atom for scattering and for absorbing x-rays changes abruptly at x-ray energies which are just sufficient to ionize a core electron. This energy is called an atomic absorption edge. Thus, one can do spectroscopy of diffracted x-rays from buried interfaces as a penetrating probe sensitive to interfacial chemistry. The oxidation state of an atom may be determined by measuring the near-edge structure of either of these cross sections; changes in chemical valence result in small shifts in ionization threshold. By measuring changes in the cross section for diffraction from an interface, two scientists (E. D. Specht and F. J. Walker) from ORNL using the National Synchrotron Light Source (NSLS) have measured the near-edge structure for an atomic layer at a buried interface and determined the oxidation state of this interfacial layer, without interference from a thick film of the same elemental composition. They have measured diffraction from the buried interface between an Al_2O_3 substrate and a 100 nm thick Cr_2O_3 film. By comparing the near-edge structure at the Cr absorption edge with that of Cr metal and Cr_2O_3 standards, they have shown that the Cr atoms at the interface are in the Cr^{+3} oxidation state.

Magnetic Resonance Imaging (MRI) Employed to Measure Two-Phase Flow

A perennial problem in the studies of multi-phase flows is the difficulty of measuring the flow fields under realistic conditions, e.g., where the volumes of bubbles are comparable with the volume of the surrounding liquid, or when comparable amounts of immiscible liquids constitute the flow. Research conducted by Dr. E. Fukushima (Lovelace Medical Foundation), and supported by the OBES-Engineering Research Program, has shown that MRI offers a feasible means for non-intrusive measurement of the distribution and velocity field in flows of immiscible liquids. This measurement method offers an important new tool for experiments dealing with multi-phase flows and hence for testing the relevant theoretical models. In turn, validated models will be used for the control of energy-related industrial processes.

Depolymerization of Teflon Studied by Laser Ablation

Research by Dr. J. Thomas Dickinson, Washington State University, supported by the Office of Basic Energy Sciences/Division of Chemical Sciences, on the interaction of laser light with polytetrafluroethylene (Teflon) in vacuum has been used to examine the evolution of neutral and ionic species emitted during irradiation of the surface. An interesting finding from this research effort is that the major neutral component formed is the monomer (C_2F_4), which occurs due to a thermally activated unzipping reaction at the surface. The ionic species present are derived from neutral decomposition products which are ionized by electron collisions in the weak plasma generated at the PTFE surface from the laser beam. A simple model has been postulated to fit the products emitted from the surface. This research presents the interesting possibility of studying the degradation of an environmental important compound whose disposal is problematic.

Scientific Awards & Recognition

An important aspect of the Basic Energy Sciences program is its ability to foster *investigator-initiated* strategic research in areas important to the Department of Energy's missions. This "bottom-up" philosophy is practiced with the realization that innovative ideas and revolutionary advancements come from informed scientists unconstrained by preconceived notions of which specific technologies will be competitive tomorrow. Important measurements of the quality of the Basic Energy Sciences program include indicators of the level of expertise of the scientists who are supported. Listed below are examples of such metrics which indicate that many of the program's principal investigators are recognized as among the best in the world.

Nobel Prize in Chemistry

Professor R. Marcus of Cal Tech has been awarded the Nobel Prize in Chemistry for 1992. Professor Marcus has made significant theoretical contributions in a variety of topical areas of great import to DOE programs and DOE supported scientists have had a major role in both the development and confirmation of these theories. In particular, the statistical theory describing unimolecular decompositions, RRKM (Rice-Ramsberger-Kassel-Marcus), has proven to be incredibly useful in describing the gas-phase dissociation of large molecules. Similarly, Marcus developed an important theory to describe electron transfer kinetics in solution, an area directly related to solar photochemical energy conversion.

The Atomic Energy Commission (AEC) supported some of Marcus' research in hot-atom chemistry in the late 1950's and early 1960's. It was during this time that the quantum mechanical treatment of activated complex theory, a treatment that led to an advanced form of RRKM, was developed. At the same time, Marcus was a frequent visitor to Brookhaven National Laboratory (BNL) where he spent several summers during the 1958-1963 period with support from the AEC. It was during this time that discussions with Dr. Norman Sutin at BNL served as a stimulus to Marcus. Eleven papers were published which carry the BNL byline, four of them with Sutin.

When Marcus started working on his electron-transfer theory in the early 1950's, there was already a strong program at BNL using radioactive isotopes to study the simplest class of electron-transfer reactions in which there is no net chemical change. In this particular instance, two different oxidation states of a ligated metal ion undergo electron transfer, for example:

$$M^*L_6^{2+} + ML_6^{3+} <=> M^*L_6^{3+} + ML_6^{2+}$$

These reactions were conveniently studied by using a radioactive isotope (designated by the *) to label one of the oxidation states and was a "natural" for a national lab at that time. The results, also carried out elsewhere as well, were surprising. Despite the apparent simplicity in that no bonds were made or broken, the exchange rates varied by many orders of magnitude. Marcus was intrigued by these early results and he soon extended his early formalism to include reactions accompanied by a net chemical change (the Marcus cross-relation). Early experimental confirmation of several theoretical predictions were provided by Sutin's group. In the late 1980's, some 25 years after it was initially proposed, the Argonne group (John Miller and Gerhard Closs) provided confirmation of a remaining prediction of Marcus theory - the inverted region - where rates decrease with increasing driving force.

Six Office of Basic Energy Sciences Researchers Elected to National Academy of Sciences; Others Deliver Lectures, Receive Awards

Six Basic Energy Sciences supported researchers were elected to membership in the National Academy of Sciences during the 130th annual meeting of the Academy on April 25-28, 1993. The Academy announcement indicates that the election of the new members was "in recognition of their distinguished and continuing achievements in original research." The six new members (and the Division providing research support) are:

1. Professor Donald J. DePaolo, University of California, Berkeley (Engineering and Geosciences)
2. Professor Tobin J. Marks, Northwestern University, (Chemical Sciences)
3. Professor Alexandra Navrotsky, Princeton University (Materials Sciences, and Engineering and Geosciences)
4. Professor Peter G. Schultz, University of California, Berkeley (Materials Sciences and Energy Biosciences)
5. Professor Charles P. Casey, University of Wisconsin (Chemical Sciences).
6. Professor Sharon A. Long, Stanford University (Energy Biosciences)

The annual meeting also included symposium talks by Basic Energy Sciences researchers. Professor Sylvia T. Ceyer of the Massachusetts Institute of Technology spoke at the Symposium: "Science at the Frontier." Professor Peter G. Schultz of the University of California, Berkeley gave one of the talks at the Symposium: "Topics of Current Interest." The research of Professor Ceyer is supported by the Chemical Sciences Division and that of Professor Schultz by the Materials Sciences Division.

The Academy also presented awards to three scientists supported by the Office of Basic Energy Sciences. Two of the awardees, are Professor F. Sherwood Rowland (University of California, Irvine) who presented the Robertson Memorial Lecture, a lecture that touches upon the international aspects of the recipient's research, and Professor Harold S. Johnston (Lawrence Berkeley Laboratory) who received the National Academy of Sciences Award for Chemistry in Service to Society. Both awards were given in recognition of the contributions made by these two gentlemen who showed that mankind's activities could affect the chemistry of the stratosphere where, in particular, release of chlorofluorocarbons and nitrogen oxides could deplete the critical and fragile ozone layer. The research of both Professors Rowland and Johnston are supported by the Chemical Sciences Division.

The third awardee is Professor Charles P. Slichter (University of Illinois) who received the Comstock Prize (jointly with Professor Erwin L. Hahn (University of California, Berkeley)) in recognition of his seminal contributions to the development and application of magnetic resonance in condensed matter, including the first experimental proof of pairing correlations in superconductors and fundamental studies in surface science and catalysis. Professor Slichter's research is supported by the Materials Sciences Division.

The prize of $10,000 (each) is awarded every 5 years "for the most important discovery or investigation in electricity, magnetism, or radiant energy; to be given to a resident of North America." The list of prior winners, including seven

Nobel Laureates, demonstrates that this is an award of great distinction. On the same day he received notification of the Comstock Prize, Professor Slichter received notice that he was awarded an Honorary Degree at the University of Waterloo in Ontario, Canada, on May 28, 1993. He presented the Convocation address.

Honors for Engineering Research Program Researcher

Professor D. D. Joseph (U. of Minnesota) has received the Brigham Medal from the Society of Rheology in recognition of his " ...superb record of accomplishments, having made major contributions to the fields of rheology; fluid mechanics, and thermal sciences." In addition, Professor Joseph was awarded an unrestricted $20,000 grant from Schlumberger Foundation, citing him " ...for his pioneering and continuing work on the sonic shear velocity within viscoelastic fluids and slurries." The Office of Basic Energy Sciences/ Engineering Research Program supports Professor Joseph's research on lubricated crude oil pipelines, aimed at reducing the pumping power needed to maintain a rapid flow of the crude oil.

Medal Awarded for Development of Atomic Number Contrast Imaging Microscope

The Materials Research Society's (MRS) Medal Award was established by the MRS to recognize a distinguished recent innovative achievement or discovery which is expected to have a major impact on the progress of any materials related field. One of the two 1992 MRS Medal Awards was presented to Dr. Stephen J. Pennycook of ORNL at the MRS Meeting in Boston on December 1, 1992, "for the development of incoherent (atomic number contrast) imaging in the scanning transmission electron microscope for direct determination of the atomic scale structure and chemistry of materials and interfaces."

Through the development of high-resolution incoherent (Z-contrast) imaging in the scanning transmission electron microscope (STEM) Pennycook achieved a major long-term goal of electron microscopy: atomic resolution in a chemically sensitive image which is directly and easily interpretable. This, in turn, constitutes a major advance for virtually every branch of materials research, where new opportunities are opened by the ability to directly associate chemical and microstructural information. The technique has already made big contributions in the areas of superconductors, semiconductors, ceramics, grain structure in metals and alloys, interfaces and catalysts. One example is Pennycook's recent imaging of striking local differences in the atomic structure of 1-2-3 superconductors when Er is substituted for Y.

Dr. Pennycook's approach departs from conventional phase-contrast high-resolution electron microscopy. The technique relies on the detection of transmitted electrons scattered through high angles. The incoherent scattering of these electrons occurs mainly at unscreened nuclei, and thus gives an image with strong atomic-number (Z) contrast, and with only minor dependence on specimen thickness and microscope defocus. A National Science Foundation Workshop on Atomic Reduction Microscopy proposed a major commitment of support for field-emission STEM instruments, a further recognition of the anticipated impact of Pennycook's work on the field. Dr. Pennycook also recently received the 1992 Kurt F. J. Heinrich Outstanding Young Scientist Award of the Microbeam Analysis Society.

Feature Interview Focuses on "Synthetic Metals"

Science Watch, a monthly publication of the Institute for Scientific Information designed to track trends and performance in basic research, highlights, in the January 1993 issue, an interview with Dr. Jack Williams of the Chemistry and the Materials Sciences Divisions at Argonne National Laboratory. The interview focuses on the world-wide research on organic superconductors and "synthetic" metals. Dr. Williams and his group at Argonne National Laboratory hold the current record of 12.8 kelvin for superconductivity in an organic charge transfer salt. This is the highest transition temperature recorded for an organic material (except for the other well known organic molecules - the fullerenes - one of which has a superconducting transition temperature of 33 kelvin). When *Science*

Watch scrutinized this field 3 years ago, Dr. Williams' group at Argonne ranked third in the world in its share of the research literature on organic superconductors - the sole American lab to make the Top Ten (see *Science Watch*, Fall 1989, page 7). *Science Watch* previously highlighted Dr. Williams' standing among the 50 most-cited chemists in the world, according to average citations per paper for the period 1984-1991.

1993 Fellows Named by ASM International

The list of 50 Fellows of ASM International (formerly the American Society for Metals) that were installed during Materials Week '93, held in Pittsburgh, Pennsylvania, on October 19, 1993, includes four researchers who received support in FY 1993 from the Office of Basic Energy Sciences. Two of the recipients are Oak Ridge National Laboratory employees. Peter J. Blau, supported by the Division of Advanced Energy Projects, received his honor for "innovative research leading to a new level of understanding of the mechanisms of friction and wear and for original contributions to the science of tribology." Dr. Blau is engaged in a research project on Novel Composite Coatings for High-Temperature Friction and Wear Control. Linda L. Horton received her award for "sustained contributions to the basic understanding of radiation effects in ferritic alloys and to pre-college educational outreach in materials science and engineering." Dr. Horton was the principal organizer for a planning workshop for the Division of Advanced Energy Projects entitled, "Innovation in Materials Processing and Manufacture: Exploratory Concepts for Energy Applications," held on March 11-12, 1993, at Oak Ridge, Tennessee. She is also funded by the Division of Materials Sciences. Two additional Materials Sciences grantees were installed as fellows: Professor Tarasankar DebRoy, Pennsylvania State University, "For pioneering fundamental research in welding and chemical vapor deposition, and for leading efforts in the mathematical modelling of welding processes"; and Dr. U. Fred Kocks, Los Alamos National Laboratory, "For exemplary leadership in the integration of physical theory and empirical phenomenology in the field of plasticity of metals and alloys."

Dr. Linda L. Horton Receives Additional Two Honors

Dr. Linda L. Horton, manager of the Basic Energy Sciences (BES) programs in the Metals and Ceramics Division of Oak Ridge National Laboratory (ORNL), was elected to a three year term (January 1993 - December 1995) as Director, Physical Sciences, of the Microscopy Society of America (MSA, previously known as the Electron Microscopy Society of America). The MSA is a national professional society composed of nearly 5,000 microscopy professionals from both the Physical and Life Sciences. Dr. Horton is one of three Directors for the Physical Sciences; the others are Dr. Philip Sklad, also of ORNL, and Dr. C. Barry Carter, University of Minnesota. Through their careers, both Drs. Sklad and Carter have been long-term recipients of BES support.

In a separate action, Dr. Linda L. Horton is one of the four nominees expected to serve a three year term as a Trustee of the ASM International. Dr. Horton is the first woman to be nominated as a trustee for the ASM International. She is also active in student outreach programs and coordinator of the pre-college education activities at the Oak Ridge National Laboratory Metals and Ceramics Division, and has served as a member of the ASM Advisory Technical Awareness Council, Nominating Committee, Editorial Committee for "Advanced Materials and Processes," and the ASM International 2,000 Committee.

Shared Research Equipment Program

The BES/Materials Sciences Division-funded Shared Research Equipment Program, SHaRE, managed by Dr. Edward Kenik, Oak Ridge National Laboratory (ORNL), and Dr. Neal Evans, Oak Ridge Institute for Science and Education (ORISE), recently completed another successful year. During FY 1992, increases in the numbers of proposals, participants, and user days were achieved relative to FY 1991: 27 proposals were accepted representing an increase of ~50 percent over FY 1991; 31 SHaRE participants and 196 user days relative to 22 participants and 153 user days in FY 1991; SHaRE research resulted in 20 publications, 16 presentations, and 6 theses.

SHaRE research was recognized with two awards at the 1992 annual meeting of Electron Microscopy Society of America (EMSA): Graduate student Ian Anderson (Cornell University and University of Minnesota) received the 1992 EMSA Presidential Scholarship for a paper based on SHaRE research; a SHaRE industrial project with Drs. Mary Grace Burke (Westinghouse) and Edward Kenik (ORNL) received the 1992 EMSA Poster Award in Physical Sciences.

The FY 1993 SHaRE Executive Committee composed of Drs. N. D. Evans (ORISE), C. B. Carter (University of Minnesota), B. Fabes (University of Arizona), E. A. Kenik (ORNL), and J. Bentley (ORNL) met in early October 1992 to review 25 proposals. This is the largest number of proposals received at the beginning of the fiscal year and included three from industry. From these proposals, 22 were accepted, 2 were referred to more appropriate ORNL user centers (Surface Modification and Characterization Facility, Neutron Scattering Facilities), and one was returned for further information. The Committee awarded $20K in travel support with an average award of $900. Several of the accepted proposals did not receive travel grants.

Two DOE National Laboratories in List of "Top U.S. Institutions in Chemistry"

The July 23, 1993, issue of *Science* contains, in the Random Samples Section, page 423, a list of 15 institutions entitled "Top U.S. Institutions in Chemistry." The Lawrence Berkeley Laboratory is ranked number 13 and Argonne National Laboratory is ranked at number 15. The rankings are based on citation impact from 1988 to 1992 in the world-wide chemical literature as compiled by *Science Watch*, a publication of the Institute for Scientific Information.

In commenting on the list, *Science* says "Perhaps the biggest surprise is Boston's Northeastern University weighing in at number seven with 7.19 citations per paper. Much of Northeastern's success can be attributed to three papers on molecular/organic ferromagnets. The papers, coauthorized by Northeastern's William Reiff, Dupont's Joel Miller, and Ohio State's Arthur Epstein, racked up a total of 380 citations." Miller and Epstein's collaborative research on molecular/organic ferromagnets was initiated with support from the Office of Basic Energy Sciences/Division of Materials Sciences. Miller is now at the University of Utah and his research and that of Epstein at Ohio State University continues to be supported by the Division of Materials Sciences.

Scientists Win American Chemical Society National Awards

The 1994 National awards for chemistry have been announced by the American Chemical Society and include a number of scientists supported by the Office of Basic Energy Sciences (BES). The BES- supported scientists and their awards are listed below.

Edward S. Yeung	Analytical Chemistry Award
Tobin J. Marks	Inorganic Chemistry Award
John A. Gladysz	Organometallic Chemistry Award
Gerard F.R. Parkin	Pure Chemistry Award
Adam Heller	Materials Chemistry Award
William H. Miller	Theoretical Chemistry Award
Gabor A. Somoraji	Distinguished Service in the Advancement of Surface Chemistry Award
Kenneth N. Raymond	Bioinorganic Chemistry Award
Gary R. Dyrkacz	Fuel Chemistry Award

Additionally, a former BES-supported scientist, Glenn T. Seaborg, was given the George Pimentel award for advancing chemical education. Vignettes of award winners appear in the fall 1993 issues of *Chemical & Engineering News*, while the presentations were made during the Fall American Chemical Society meeting held in Chicago.

Since the establishment of the Organometallic Chemistry Award by the Dow Chemical Foundation in 1983, eight of the nine awards which have been presented (including Gladysz) were won by Basic Energy Sciences/Chemical Sciences Division supported investigators. Previous Office of Basic Energy Sciences-supported recipients were Charles Casey (1991), John Bercaw (1990), Tobin Marks (1989), Robert Grubbs (1988), Peter Vollhardt (1987), Robert Bergman (1986), and Richard Schrock (1985).

Acta Metallurgica Gold Medal Award to Professor William D. Nix

Acta Metallurgica has announced that the recipient of its 1993 Acta Metallurgica Gold Medal Award is Professor William D. Nix of Stanford University. The Acta Metallurgica Gold Medal is an international award, established in 1974, that recognizes outstanding ability and leadership in materials research. Professor Nix has been a major force in establishing and maintaining the Department of Materials Science and Engineering, which he chairs, at Stanford University. His research interests have focused on theoretical and experimental aspects of the high-temperature mechanical behavior of crystalline materials. More recently, he has concentrated on studying the mechanical behavior of thin films. He also made major inroads through his experiments and modeling of the phenomena and mechanisms of creep deformation and fracture. He has authored or co-authored 224 scientific publications, including a textbook, "The Principles of Engineering Materials." Professor Nix is also a fellow of The Metallurgical Society. The Gold Medal was be presented to Professor Nix at the meeting of The Metallurgical Society in Pittsburgh during the week of October 17. Professor Nix is a grantee of the Office of Basic Energy Sciences/Materials Sciences program.

Energy Biosciences Division Grantees Receive Honors

At the annual meeting of the American Society of Plant Physiologists in Minneapolis on August 1, 1993, four awards were made to individuals who have made outstanding contributions to the discipline of plant physiology. One of these was to a foreign investigator. The other three were to domestic investigators, all of whom either had Energy Biosciences support, or continue to receive it. The Charles Reid Barnes Life Membership Award was given to Dr. Frank Loewus of Washington State University, who is now Emeritus and who had previously been an Energy Biosciences grantee. The second award, The Charles Albert Shull Award, was given to Dr. Ilya Raskin of Rutgers University for his outstanding investigations. He is currently an Energy Biosciences grantee. The third award, the Martin Gibbs Medal, was given to Christopher R. Somerville of the Michigan State University/Department of Energy/Plant Research Laboratory for his leadership in implementing new research directions in plant physiology.

University of Chicago Award for Distinguished Performance Goes to Dr. Berkowitz

One of the pioneers of modern photoionization mass spectrometry and high-temperature photoelectron spectroscopy, Dr. Joseph Berkowitz, has received the highest award offered at Argonne National Laboratory, the University of Chicago Award for Distinguished Performance. The essence of the award citation notes that Dr. Berkowitz' work has had a major impact on the fields of chemical physics and physical chemistry. His imaginative choices of experimental techniques and interpretation of data have led to new insights into chemical bonding. In addition to broadening an understanding of chemical structure and of thermodynamic stability of important substances, his work has increased our knowledge of a broad range of phenomena, including combustion, silicon-chip production, and interstellar chemistry. Dr. Berkowitz is supported by the Office of Basic Energy Sciences/Chemical Sciences Division and his first observation of the COOH radical was a recent significant achievement.

Chemist Receives Calorimetry Conference Award

Dr. John M. Simonson, supported by the Office of Basic Energy Sciences/ Division of Chemical Sciences at the Oak Ridge National Laboratory, was named the 1993 recipient of the prestigious Sunner Award. This award is sponsored by Hart Scientific Co. and is presented each year at the Calorimetry Conference to a scientist under the age of

40 who is establishing a high standard of consistent superior performance in the thermochemistry and thermodynamics research area. Dr. Simonson received a plaque, an honorarium, and presented the plenary lecture at a meeting of the Calorimetry Conference.

Division of Materials Sciences-Supported Student Wins 1993 Nottingham Prize

Ms. Anna Swan, a graduate student in the Physics Department at Boston University, has been awarded the 1993 Nottingham Prize at the 53nd Annual Physical Electronics Conference held at Rensselaer Polytechnic Institute, Troy, New York, in June 1993. The Nottingham Prize is awarded to the best student paper presented at each conference and has achieved a distinguished reputation due to the successfulness of past recipients and to the quality of the competition.

Ms. Swan's research, supported by the Office of Basic Energy Sciences/ Materials Sciences Division, involves the use of metastable helium atom scattering to determine magnetic spin ordering on an insulator surface. This research produced the first definitive measurement necessary to help solve this long-standing problem in surface science. The results and the new technique have implications to a range of surface science studies, particularly in the electronics industry where electron spin ordering is seen as a key feature in further minaturization of electronic devices.

Researcher Elected International Vacuum Society President

Professor Theodore E. Madey, a Basic Energy Science, Chemical Sciences-funded researcher from Rutgers University, has been elected President of the International Vacuum Society. The International Vacuum Society represents scientists with a common interest in the areas of surface physics and chemistry. Election to this position represents recognition by his peers of his significant contributions to the understanding of the physics and chemistry of surface processes.

Dr. Gary McVay Receives an Honorary Degree

Dr. Gary L. McVay, Pacific Northwest Laboratories, received an honorary "Professional Degree of Ceramic Engineer" from the University of Missouri - Rolla, at the commencement exercises held in Rolla, Missouri, on May 15, 1993. According to the letter received from John T. Park, Chancellor, University of Missouri - Rolla: "Each year the University of Missouri - Rolla, awards a limited number of professional degrees to persons who have made important contributions to the engineering or science profession. A predominant criterion for selection of the individual is a distinguished career, such as yours, in engineering or science." Dr. McVay is the Laboratory Coordinator for Division of Materials Sciences programs at the Pacific Northwest Laboratories and Manager of the Laboratories' Materials Sciences Department.

American Welding Society Conferred Honors to Division of Materials Sciences-Funded Students

At its annual convention held in Houston this past April, the American Welding Society conferred top awards in the student poster competition to all three students of Materials Sciences grantee, Professor T. DebRoy of the Pennsylvania State University. Professors Dan Madey and Kamlesh Mundra received first prize with their poster entitled "Oxygen Dissolution and its Effect on the Fluid Flow and Heat Transfer in Weld Pools." Professor Carina Onneby's poster, entitled "Nitrogen Dissolution in the Weld Pools" and Mundra's other poster, entitled "A Two-temperature Model of Nitrogen Dissolution in the Weld Pool" tied for second place.

Division of Chemical Sciences Grantee Delivers Commencement Address

Professor Larry Curtis in the Department of Physics and Astronomy of Toledo University was accorded an unusual distinction by being selected to deliver the commencement address to the University graduates. Curtis, who received his B.S. degree from the University and his Ph.D. from the University of Michigan, is known internationally for his research on atomic structure and is supported by the Office of Basic Energy Sciences/Division of Chemical Sciences. He holds visiting professorships at Princeton University, the Research Institute for Physics in Stockholm, the Universities of Lund and of Uppsala in Sweden, the University of Aarhus in Denmark, the University of Lyon in France and the Free University of Berlin in Germany. In his address, he stressed the virtues of receiving an education from a small research oriented university where research and teaching faculties are not separated.

Citation Classic

Professor Gregory Stewart, University of Florida, has been asked to write a *Citation Classic* "for publication in *Current Contents*" describing, in an anecdotal style, how his 1984 *Reviews of Modern Physics* article on heavy fermions came to be. The review, "Heavy Fermion Systems," has been so highly cited as to be designated a "classic." Stewart's research on heavy Fermion materials is supported by the Office of Basic Energy Sciences, Division of Materials Sciences.

Chemical Sciences Division Grantee to Receive Honorary Degree

Professor Mostafa El-Sayed of the University of California, Los Angeles received the Doctor Philosophiae Honoris Causa from the Hebrew University of Jerusalem, Israel at an annual convocation held in June 1993, in Jerusalem. The citation noted "singularly outstanding contributions to the field of photochemistry and photobiology and, in particular, to the elucidation of the mechanism of vision. Your important role in bringing about international scientific cooperation, your special interest in the progress of science in the third world and your close research ties with the community of physical chemistry in Israel and at the Hebrew University are deeply appreciated".

Professor El-Sayed did his undergraduate work at Ein Shams University, Cairo, Egypt followed by graduate work at Florida State University with Michael Kasha. Following several post-doctoral positions he joined the faculty of the University of California/Los Angeles in 1961. He has been a member of the National Academy of Sciences since 1980. Professor El-Sayed has been supported by the Chemical Sciences Division since 1978.

Chemical Sciences Division Grantee Appointed Distinguished Scientist at the University of Tennessee

Professor Peter T. Cummings has recently been selected to become a University of Tennessee-Oak Ridge National Laboratory Distinguished Scientist. He is currently a member of the Chemical Engineering faculty at the University of Virginia, where he has been supported by the Chemical Sciences Division for research to understand and develop predictive tools for the thermodynamic properties and phase equilibria of mixed solvent electrolytes. He will join the University of Tennessee faculty in January 1994. He has collaborated with Oak Ridge National Laboratory groups in Chemistry and Materials Sciences on molecular simulations of supercritical aqueous solutions which is relevant to waste processing.

This is the second Chemical Sciences principal investigator to be appointed to a University of Tennessee-Oak Ridge National Laboratory Distinguished Scientist position. Professor Georges Guiochon, who is a world renowned practitioner and theorist in chromatographic separations, was so appointed in 1987. He was formerly a professor at the University of Paris, and later at Georgetown University where he was supported for research on chromatographic detectors for low concentration solutes important to characterizing fossil fuels, synthetic fuels, and waste streams related to energy production.

Alexander von Humboldt Award Received by Chemical Sciences Division Investigator

Professor Kenneth N. Raymond, a Chemical Sciences-funded investigator at the University of California/Lawrence Berkeley Laboratory is the recipient of a prestigious Alexander von Humboldt Research Award to study at the

University of Bochum with Professor Dr. Karl Wieghardt. This is in recognition of his outstanding studies in the chemistry of actinide complexing and sequestering agents both for the decorporation of actinides, specifically plutonium, and for possible application to the separation of actinides from the processing streams of nuclear materials. Professor Raymond received the E. O. Lawrence Award in chemistry in 1984.

Argonne Scientist Receives Senior Humboldt Award

Dr. James R. Norris, a Senior Chemist in the Chemistry Division at Argonne National Laboratory, has been awarded an Alexander von Humboldt U.S. Senior Scientist Award. Sponsored by the Alexander von Humboldt Foundation of the Federal Republic of Germany, the award will enable Norris to pursue research in photosynthesis at the University of Stuttgart for six months in 1993. Norris received the Department of Energy E. O. Lawrence Award in 1990 for his research contributions in the area of photosynthesis.

Two Humboldt Foundation Awards and a Scholar Award to Scientists at the University of Illinois -Materials Research Laboratory

Professor Robert Averback and Professor Ralph Simmons, each have been awarded the Distinguished Senior U.S. Scientist Award from the Humboldt Foundation to carry out research in Germany. Professor Averback will work at three institutions: University of Augsburg, Hahn-Meitner Institute in Berlin, and the Forschungszentrum-Julich. His activities at the three institutions will center on radiation effects in solids starting in January 1993 for a year.

Professor Simmons began his year in September 1992 at the University of Munich to carry out research on monochrometers suitable for use on intense light sources such as the Advanced Photon Source under construction at the Argonne National Laboratory.

Professor Walter G. Klemperer has been selected as a 1992 University of Illinois Scholar in recognition of his excellence in research and teaching. This award carries an annual award of $12,000 for each of 3 years to facilitate his research. Professor Klemperer is an outstanding and award-winning scientist supported by the BES/Division of Materials Sciences through the Materials Research Laboratory at the University of Illinois.

Humboldt Research Award Awarded to Oak Ridge National Laboratory Scientist

Dr. Man H. Yoo, Oak Ridge National Laboratory, has been awarded a Humboldt Research Award for Senior Scientists by the Alexander von Humboldt Foundation, Germany. Humboldt Awards are presented annually to scientists throughout the world; Dr. Yoo has received one of less than sixty awards presented to senior scientists in the United States. These awards are intended to promote long-term specialized cooperation between scientists in Germany and other countries. The Humboldt Award recognizes Yoo's achievements in intermetallics research. Dr. Yoo has been supported by the Division of Materials Sciences, Basic Energy Sciences Program, at Oak Ridge throughout his career. During the past eight years, his research has focussed on establishing a theoretical basis for understanding and improving the mechanical properties of intermetallic alloys. The financial grant associated with the Humboldt Award will allow Dr. Yoo to spend twelve months at German research institutes, beginning in fiscal year 1994.

Council on Materials Science Report Cited as Inspiration for Award-Winning Ceramic Research

On April 19, 1993, the Orton Memorial Lecture at the American Ceramic Society Meeting, Professor J. Derek Birchall, Professor of Inorganic Chemistry of the University of Keele, Staffordshire, United Kingdom, cited a statement in a 1978 report of the Council on Materials Science as the motivation that led him to his award-winning research on ceramics with improved reliability. The Edward Orton Jr. Memorial Lecture is given each year at the spring meeting of the American Ceramic Society in recognition of distinguished research in some area of ceramic science and technology. Professor Birchall's research group is noted for their invention of Saffril aluminum and zirconium oxide fibers, ceramic binders, macro-defect-free cement and macro-defect-free technology for the processing of advanced ceramics. The Council on Materials Science is supported by the Department of Energy's Office of Basic Energy Sciences/Division of Materials Sciences to assess the state-of-the-art in various fields of material science. The Council convenes panels of experts to review a field and to publish the result of their findings in the professional literature. The 1978 report cited by Professor Birchall was published as "Basic Research Needs on High Temperature Ceramics for Energy Applications," in a 1980 issue of *Materials Science and Engineering*. The panel which prepared that report was chaired by Professor H. K. Bowen of the Massachusetts Institute of Technology.

Scientists Honored by Catalysis Society

Professor Wolfgang M. H. Sachtler of Northwestern University received the Houdry Award from the Catalysis Society of North America on May 3, 1993. The Houdry Award is presented biannually to an individual who has made outstanding contributions to the field of industrial catalysis.

Professor Mark A. Barteau of Delaware University received the Emmett Award, also presented biannually, for new fundamental contributions to the field of catalysis. The Emmett award is restricted to researchers who, besides having made significant contributions, have not reached 43 years of age. Both, Drs. Sachtler and Barteau, are supported by the Office of Basic Energy Sciences/Division of Chemical Sciences.

Oak Ridge Scientist Elected Corporate Fellow

Dr. Lynn A. Boatner, Solid State Division, Oak Ridge National Laboratory, was elected to Corporate Fellowship, Martin Marietta Energy Systems, Inc. on March 1, 1993. Corporate Fellowship is one of the highest honors conferred by Martin Marietta Energy Systems, Inc. and is given only to those rare individuals whose contributions have been both significant and continually high over a number of years. Dr. Boatner was cited for his continuing accomplishments in the field of materials synthesis, rapid solidification, and technology. Dr. Boatner's research is supported by the Office of Basic Energy Sciences/Division of Materials Sciences.

Three Basic Energy Sciences Grantees Elected to United States National Academy of Engineering

Professor Jerome B. Cohen, an Office of Basic Energy Sciencs/Materials Sciences Division grantee from Northwestern University has been elected to membership in the United States National Academy of Engineering. His citation states "For contributions to X-ray diffraction of materials, including residual stress, ceramics, and catalysts."

Chemical Sciences Division Investigator, Professor Jan D. Miller, Department of Metallurgical Engineering, University of Utah, has been elected to the National Academy of Engineering. This prestigious recognition honors those who have made important contributions to engineering theory and practice. Dr. Miller's research efforts supported by the Chemical Sciences Division involve the fundamental investigation and characterization of the interfacial region of nonsulfide minerals and surfactant molecules used in floatation separations. The National Academy of Engineering has 1684 U.S. members and 142 foreign associates.

Professor Manfred Morari (California Institute of Technology) has been elected to the National Academy of Engineering. Professor Morari, currently the Chairman of the Chemical Engineering Department at California Institute of Technology, was cited for his contributions to the foundations of chemical process control, i.e., research carried out under Basic Energy Sciences/Engineering Research Program sponsorship.

K.A. Gschneidner, Jr. Symposium Held in Kyoto

A special symposium entitled "The K.A. Gschneidner, Jr. Symposium," was held on June 1-5, 1992, at the Rare Earths '92 conference in Kyoto, Japan. Professor Gschneidner is an investigator in the Materials Sciences program at the Ames Laboratory and holds the rank of Distinguished Professor at Iowa State University. The citation for this Symposium Dedication to him stated it was in "honor of his meritorious service to rare earth sciences and industries." Professor Gschneidner has been the recipient of many other honors including the William Hume-Rothery Award of the Metallurgical Society, the Burlington Northern Award for Excellence in Research from Iowa State University, and the Frank H. Spedding Award for distinguished contributions for rare earth science from the Rare Earth Research Conference, Inc. Professor Gschneidner has been elected a Fellow to both the Minerals, Metals and Materials Society and the American Society for Materials International, and one of his research papers was named a "citation classic" by the Institute for Scientific Information.

Stanford Synchrotron Radiation Laboratory Scientist Received Two Honors

Dr. Z. X. Shen, a Stanford Synchrotron Radiation Laboratory faculty member with a joint appointment in the Stanford University Department of Applied Physics, has been announced as a co-recipient of the annual Overseas Chinese Physicist Association award. The award citation acknowledges his pioneering studies of highly correlated systems using angle-resolved photoemission and for the resulting elucidation of the nature of high-Tc superconductors, Mott insulators, ferromagnetic systems, and fullerenes.

Dr. Shen was also recently selected as a Sloan Fellow by the Alfred P. Sloan Foundation; his primary research program is centered on Stanford Synchrotron Radiation Laboratory's multi-undulator beam line.

Professor Simon Moss Receives the 1993 David Adler Lectureship Award

Professor Simon Moss of the University of Houston was selected as the 1993 winner of the David Adler Lectureship Award by the American Physical Society for "outstanding contributions to the understanding of the structure and transformation behavior of new materials, including ordered metallic alloys, amorphous metals and semiconductors, quasicrystals, oxide superconductors and fullerenes." Professor Moss is supported by the Office of Basic Energy Sciences/Division of Materials Sciences for his research in X-ray and neutron studies of glasses and liquids.

Torgersen Named Editor of *Reviews of Geophysics*

The President of the American Geophysical Union appointed Tom Torgersen to a 4-year term as an Editor of the journal *Reviews of Geophysics*, a multidisciplinary journal of the American Geophysical Union. Torgersen is an Intergovernmental Personnel Act employee in the Office of Basic Energy Sciences/Geosciences program.

Chemical Sciences-Supported Scientists Receive Department of Commerce Silver Medal Award

Two scientists, Drs. Michael Kelley and Jabez McClelland, supported by the BES/Division of Chemical Sciences were among the group of National Institute for Science and Technology scientists recognized by the Department of Commerce in 1992. Both scientists were recipients of the Silver Medal Award, "the second highest honorary award given by the Department and granted by the Secretary of Commerce (Ms. Barbara Franklin) for meritorious contributions of unusual value to the Department or the Nation." In this case, Kelley and McClelland were recognized for "performing an extraordinary series of experiments utilizing polarized electron, atom and laser beams to study the electron-atom collision process at its most fundamental level." Chemical Sciences support for this project was initiated in 1982 and over the past decade the needed techniques were advanced and the knowledge acquired to the point where the "complete" collision experiment involving electrons and sodium atoms was ultimately brought to fruition. The agreement with theory was excellent and sets a benchmark for collision experiments.

American Physical Society Prize Awarded to a Division of Materials Sciences Principal Investigator

The American Physical Society (APS) has announced the award of the 1993 High Polymer Physics Prize to Professor Benjamin Chu of the Departments of Chemistry and Materials Science and Engineering at the State University of New York at Stony Brook. Professor Chu is supported by the BES/Materials Sciences Division for X-ray scattering and instrument development in polymer research. The award citation reads: "For his matchless experimental studies of static and dynamic light scattering and X-ray scattering in polymer solutions and critical mixtures." The Prize was bestowed on March 22, 1993, at the APS National Meeting in Seattle, Washington. This prize is endowed by the Ford Motor Company. Professor Chu is supported by the Division of Materials Sciences in the Office of Basic Energy Sciences for his research on the phase transitions in polymer blends and structure of ionomers.

This is the second consecutive year that this Prize was given to a Materials Sciences principal investigator. The 1992 Prize was awarded to Professor Philip Pincus of the University of California at Santa Barbara.

Chemical Sciences Investigators Appointed to Analytical Chemistry's Instrumentation Advisory Panel

Two investigators from the BES/Division of Chemical Sciences have been appointed to three year terms on the Instrumentation Advisory Panel of the premier journal in analytical science, *Analytical Chemistry*. These investigators are J. Michael Ramsey, Oak Ridge National Laboratory, and Therese Cotton, Ames Laboratory. This American Chemical Society publication disseminates basic and applied findings in analytical science to the scientific community at large. The current Editor of *Analytical Chemistry*, Royce W. Murray, is also supported by the Division of Chemical Sciences. The role of the Instrumentation Advisory Panel is to advise the editor on instrumentation articles for the journal and to promote interest in various chemical measurement systems.

Fourteen Scientists Supported by Basic Energy Sciences (BES) Elected Fellows of the American Physical Society (APS)

The APS has announced the election to Fellowship in the Society of fourteen BES supported researchers. The fourteen were elected from the four Society subunits most relevant to BES supported research - Chemical Physics, Condensed Matter Physics, Materials Physics, and High Polymer Physics. A total of 54 new Fellows were elected from the four subunits. Formal awarding of the Fellowship Certificates took place during the Society's March meeting in Seattle, Washington, March 22-26, 1993. The names and citations of the awardees (which will be published in the March, 1993 issue of *APS News*) are:

Dr. Alexei A. Abrikosov, Argonne National Laboratory
"For his predictions of the existence and properties of the vortex state in Type II superconductors."

Professor Pulak Dutta, Northwestern University
"For his elucidations of the structures and phase transitions of lipid monolayers."

Professor Edward A. Stern, University of Washington
"For his development of extended X-ray fine structure and measurements on metals, alloys, and molecules."

Dr. Joe David Thompson, Los Alamos National Laboratory
"For his contributions to the understanding of transport, magnetic and thermodynamic properties of novel materials, particularly those displaying strong electronic correlations, and for pioneering high pressure studies of these materials."

Professor Eric J. Amis, University of Southern California
"For the excellence of his contribution toward the understanding of dynamics of polymer solutions and gels, and in crystalline growth."

Professor John Edward Fischer, University of Pennsylvania
"For seminal studies of layered solids and for developing a unified approach to phase equilibria in guest-host systems with competing interactions such as graphite intercalation compounds, polyacetylene, and fullerenes."

Dr. Gary Lee Kellogg, Sandia National Laboratories/Albuquerque
"For pioneering contributions to understanding the structure, migration, clustering and chemical reaction processes of atoms on surfaces."

Dr. Terence Edward Mitchell, Los Alamos National Laboratory
"For notable contributions to the understanding of the relationship between structure and properties of materials, particularly with regard to the use of transmission electron microscopy to reveal the defect structures."

Dr. Marie-Louis Saboungi, Argonne National Laboratory
"For innovative research into the structure of liquid metals, semiconductors and molten salts which has led to profound changes in the way we view the liquid state of matter."

Professor Paul F. Barbara, University of Minnesota
"For his innovative studies of ultrafast proton and electron transfers, isomerization reactions, and dynamic solvent effects"

Professor Hai-Lung Dai, University of Pennsylvania
"For developing novel laser spectroscopic techniques and the observation of novel properties of exotic chemical species such as transient, weakly bound, and reactive molecules in gases and molecules absorbed on surfaces".

Dr. Thomas H. Dunning, Jr., Pacific Northwestern Laboratory
"For contributions to the development of methods and techniques for electronic structure calculations on molecules and for applications to fundamental chemical problems in atmospheric chemistry, laser chemistry, and combustion chemistry"

Professor John T. Yates, Jr., University of Pittsburgh
"For the study of chemical and dynamical behavior of chemisorbed species on single crystal surfaces"

Professor Katja Lindenberg, University of California/San Diego
"For her fundamental contributions to nonequilibrium statistical mechanics and the theory of stochastic processes toward the understanding of the evolution of coupled nonlinear systems of importance in physical applications"

<u>Three Materials Sciences-Supported Scientists Receive Awards at Brookhaven National Laboratory</u>

Drs. Per Bak, Peter Takacs, and Masaki Suenaga are among five Brookhaven National Laboratory scientists honored as recipients of the Laboratory's Distinguished Research and Development Award. Each researcher received a commemorating plaque and a monetary award at a ceremony hosted by BNL Director, Nicholas Samios on December 14, 1992. Dr. Per Bak, Senior Physicist, Physics Department was cited for his pioneering work on the phenomenon of self-organized criticality; Dr. Peter Takacs, Physicist, Instrumentation Division, for his contributions to the metrology of mirror surfaces; and Dr. Masaki Suenaga, Senior Metallurgist, Department of Applied Science for his materials science research and engineering of superconducting materials, especially niobium-tin. The three honorees are supported by the BES/Division of Materials Sciences.

Chemical Sciences Researchers Win Prestigious Analytical Chemistry Awards

Chemical Sciences investigator, Edward S. Yeung, Ames Laboratory, has been awarded the Pittsburgh Analytical Chemistry Award from the Society for Analytical Chemists of Pittsburgh. This award recognized Ed Yeung's research in analytical separations and spectroscopy. The award was presented in March 1993 at the 44th Pittsburgh Conference on Analytical Chemistry & Applied Spectroscopy.

Chemical Sciences investigator, Robert S. (Sam) Houk, Ames Laboratory, has been awarded the Maurice F. Hasler Award. This award is sponsored by Applied Research Laboratories and administered by the Spectroscopy Society of Pittsburgh. The award recognizes Sam Houk's research in inductively coupled plasma mass spectrometry and its use for analysis of metals. The award was presented in March 1993 at the 44th Pittsburgh Conference on Analytical Chemistry & Applied Spectroscopy. Previous winners of this prestigious award include George Pimentel, Sir Alan Walsh (the inventor of Atomic Absorption Spectroscopy), Karl Siegbahn (inventor of X-ray Photoelectron Spectroscopy), and Velmer Fassel (inventor of Inductively Coupled Plasma Atomic Emission Spectroscopy).

Dr. Houk was also selected as the 1993 recipient of the American Chemical Society, Division of Analytical Chemistry **Award in Chemical Instrumentation**, sponsored by the Dow Chemical Company Foundation. This award recognizes Sam Houk's efforts in advancing the chemical instrumentation of inductively coupled plasma mass spectrometry through his fundamental research in this area. The award was presented in August 1993 at the National ACS meeting in Chicago. Previous winners of this prestigious award include Jim Winefordner (atomic fluorescence spectroscopy), Ed Yeung (laser spectroscopy) and Velmer Fassel (inductively coupled plasma atomic emission spectroscopy), who have also been supported by the Division of Chemical Sciences.

Chemical Sciences Principal Investigator Wins Physics Prize

University of Southern California Professor Curt Wittig has been informed that he is the recipient of the 1993 Herbert P. Broida Prize awarded annually by the American Physical Society to recognize outstanding advancements in the fields of atomic, molecular or chemical physics. The prize cited Professor Wittig "For his pioneering work in developing the field of photoinitiated reactions in weakly-bonded species to study aligned/oriented reactions in the molecular frame and his seminal contributions to the field of state-to-state unimolecular reactions." Professor Wittig has been supported by the BES/Chemical Sciences Division since 1985 for the study of the dynamics of gas phase reactions related to combustion.

Chemical Sciences Researchers Win Water Chemistry Award

Two investigators funded by BES/Chemical Sciences were chosen to receive the Second Annual Paul Cohen Memorial Award from the International Water Conference (IWC). At the 1991 IWC annual meeting (the 53rd.) in Pittsburgh, Drs. J. M. Simonson and D. A. Palmer of the Oak Ridge National Laboratory presented a paper entitled "An Experimental Study of the Volatility of Ammonium Chloride from Aqueous Solutions to High Temperatures". This was deemed the most precise and innovative paper at the conference. The authors received an inscribed copy of the ASME Handbook on Water Technology for Thermal Power Systems at a ceremony during the opening session of this year's IWC in Pittsburgh on October 19, 1992. This research achievement of Simonson and Palmer is highly regarded by all those who work on water chemistry in steam systems and contend with the corrosion problem of ammonium chloride.

Investigators Elected to the Rank of Fellow of the American Association for the Advancement of Science (AAAS)

Professor Howard K. Birnbaum of the University of Illinois Materials Science Laboratory (MRL), was elected to the rank of a Fellow of the AAAS. The honor was presented for "dedicated teaching, for outstanding research on hydrogen effects in metals, for perceptive administration of research, and for able service to the MS&E profession in the United States." He is program coordinator for BES/Materials Sciences sponsored program at the MRL. The formal presentation was in Boston on February 14, 1993.

Professor Kenneth S. Suslick, University of Illinois Materials Research Laboratory (UIMRL), was also honored by the AAAS by election to the rank of AAAS Fellow. Professor Suslick was cited for his research on the chemical effects of high intensity ultrasound. Professor Suslick, who is a principal investigator on a BES/Division of Materials Sciences project at the UIMRL, also received his certificate and rosette at the annual Fellows Forum as a part of the AAAS Annual Meeting.

Dr. Stan David, ORNL researcher and leader of the ORNL Welding Science Program, was also named Fellow of the American Association for the Advancement of Science. Dr. David was honored for his "significant advancement of welding science and technology through original and definitive research and for continued leadership and outstanding service to the national and international welding research community".

Chemical Sciences Division Grantee Recognized for Contributions to Combustion Research

Professor Jack B. Howard received the Bernard Lewis Gold Medal at an International Combustion Symposium in Australia. The medal has been awarded every two years since 1958 and recognizes major research contributions in the field of combustion. The award to Professor Howard cites his "brilliant research in the field of combustion particularly on the kinetics of soot formation and coal pyrolysis."

The research on soot formation has been supported by the Chemical Sciences Division since 1984 and has recently attracted increased attention because of Professor Howard's identification of the fullerenes, C_{60} and C_{70}, in soot. The fullerenes themselves have attracted a great deal of popular attention because of their unusual properties. Their discoverer, Professor Richard Smalley, also supported by the BES/Chemical Sciences Division, was a recipient of a 1991 Lawrence Award. Although fullerenes have been suspected to be constituents of soot for some time, the work by Professor Howard has demonstrated unequivocally their existence and the conditions for their formation. Under optimum conditions, up to 9% by weight of the soot produced is in the forms of C_{60} and C_{70}.

Technology Transfer Activities

Integration with U.S. Industry

There is an unfortunate myth that today's science is "long-term" and will only benefit our grandchildren. The Basic Energy Sciences program has demonstrated the ability to adapt quickly to support work aimed at understanding potential new technologies. It is not surprising that many of the most scientifically advanced, state-of-art technologies result from the direct transfer of basic research results to industry, and happen too rapidly to follow the traditional linear model of innovation. Given below are some examples of new technologies springing up directly from basic research in a short period of time, and the types of direct interactions between the Basic Energy Sciences program and industry which foster such innovations.

<u>Nano Instruments -- A Successful Spin-Off from a Basic Energy Sciences-Supported Program</u>

Development of instrumentation for a Basic Energy Sciences-supported program at the Oak Ridge National Laboratory led to the founding of the Nano Instruments, Inc., located in Knoxville, Tennessee. Nano Instruments, Inc., is a small business founded in 1984 to produce the "Nano Indenter" mechanical-property microprobe, a sophisticated instrument that characterizes the mechanical properties of materials on the nano (or submicron) scale. It is clear that this instrument was developed ahead of its time, and its applications now cover a wide spectrum of scientific disciplines. Its applications today include nano-crystalline materials, thin films, and composite materials.

Nano Instruments has grown to five employees and has sales of over one million dollars in 1992. The company credits Basic Energy Sciences for much of its success and marketing position. Research performed by Warren Oliver of Oak Ridge National Laboratory, and J. B. Pethica of Oxford University resulted in a patented testing technique for which the rights were waived to the inventors. The testing technique was commercialized through Nano Instruments, Inc. and has placed the company in a unique marketing position. Oliver and Pethica are the founders of Nano Instruments; Oliver is the President of the company.

Approximately thirty-five "Nano Indenters" have been sold to customers around the world, including several in Europe. The larger industrial customers include: International Business Machines, Motorola, Kodak, General Motors, and Engelhart. Nano indenters are in use at three national laboratories and a number of universities including: Stanford, Wisconsin, and Cornell. In addition to his activities with Nano Instruments, Inc., Oliver continues to perform research supported by Basic Energy Sciences at Oak Ridge National Laboratory. Research involving the Nano Indenter is the subject of a number of users under the Shared Research Equipment program and is integral to microcharacterization efforts in both the alloy and ceramics composite research programs.

<u>*Business Week* Highlights Waste-to-Fuel Venture</u>

The conversion of paper-mill sludge into clean-burning fuel through the ventures of Quadrex Corporation of Gainesville, Florida, was reported in the October 19, 1992, issue of <u>*Business Week*</u>. The heart of the process is the Office of Basic Energy Sciences/Energy Biosciences-supported discovery of a bioengineered bacterium that turns environmental waste from paper mills into ethanol. Quadrex Corporation is joining with Bionol Corporation to build a series of plants to achieve an annual production of more than 100 million gallons of fuel-grade ethanol, approximately 10% of the current U.S. production.

The technology developed through a research grant to the University of Florida is being commercialized in upstate New York and elsewhere. Quadrex and BIONOL Corporation have decided to build a plant next to a paper production plant in Glens Falls, N.Y., that will be able to accomplish two things. One is the ridding of the system of pulp waste that is an environmental contaminant. The other is the production of ethanol from the waste which can be used as a fuel additive, Some 1,100 tons of wet waste a day are estimated to emerge from 300 pulp plants and 600 paper mills daily across the country. Such technology has the dual advantage of eliminating waste and generating an energy source, in this case ethanol. The companies anticipate building several plants to perform the function. The research carried out by Dr. Lonnie Ingram of the University of Florida produced a bacterium through genetic engineering that could convert different polysaccharide wastes, such as occur in paper pulp effluents, into ethanol. The achievement was awarded the U.S. Patent Office's 5,000,000th patent. The company that received the material and developed it was BioEnergy International of Gainesville, Florida.

New Company Established from Division of Energy Biosciences Support

Another example of the passing forward of techniques and knowledge generated by Energy Biosciences Division support into commercial development recently occurred in Georgia. A new service company is in the process of being established, known as ANN. The company is based on procedures developed at the University of Georgia's Complex Carbohydrate Research Center. The process involves rapidly converting complex data emerging from analytical efforts into useful knowledge. This process can save literally hundreds of hours of labor and substantial money on the part of users. The basis of the company's service is a neural network computer program into which is fed raw analytical data from mass spectrographs, nmr spectrographs or other instruments. The process is based on utilizing accumulated data from known structures with which to compare data from unknown compounds. While the comparisons may sometimes yield exact identification of unknowns, in most cases the program will give indications of many structural characteristics of unknown compounds and, hence, make future determination of the full structure much easier.

New Catalyst Draws Commercial Interest

In 1991, BES-supported researcher Professor Vannice at Pennsylvania State University reported the serendipitous discovery of a new low temperature CO oxidation catalyst. This catalyst which consists of gold supported on titania is capable of oxidizing CO at near ambient temperatures. Pennsylvania State is currently negotiating agreements with both Air Products Chemicals Company and the Johnson Matthey Company to explore commercial applications for this catalyst. Interest in this catalyst is for the warm-up stage in auto exhaust catalysis and in cleaning up trace CO and O_2 contaminants in CO_2 for laser applications.

A unique feature of this catalyst is that the high activity is a result of the strong interaction between the active metal and the support. Professor Al Vannice was one of the discoverers of this strong metal support interaction (SMSI) in the late 1970s. The SMSI effect has been the subject of considerable study for its potential in synthesis gas and hydrogenation applications. This collaboration may result in the first application of the SMSI effect in oxidation catalysis.

Software for Molecular Modeling on Massively Parallel Computers

Pacific Northwest Laboratory and Daresbury Laboratory, one of the Science & Engineering Research Council laboratories in the United Kingdom, have announced a formal collaboration to foster the development of a new generation of molecular modeling software for massively parallel computers. The goal of the collaboration is to develop algorithms for computational chemistry which will take full advantage of the massively parallel computers currently under development both here and abroad. The collaboration will focus on three broad areas of computational molecular science: the electronic structure of molecules, the electronic structure of periodic solids, and molecular dynamics simulations. Both laboratories have established research programs in these areas, have collaborated informally in the past, and are now formalizing this relationship. The two laboratories plan a series of staff exchanges to foster the sharing of expertise, to avoid duplication, to promote timely access to the latest hardware and software (both scientific applications codes and programming tools), and to further the awareness and use of new applications in computational science in the U.S. and in Europe. The collaborative program will be managed by Dr. Martyn F. Guest, group leader of the High Performance Computational Chemistry Group at the Pacific Northwest Laboratory. This collaboration will complement and enhance the collaboration established last year between Pacific Northwest Laboratory, Argonne National Laboratory, and five companies (Allied-Signal, Amoco, DuPont, Exxon, and Phillips) to develop software for a computational "grand challenge" in environmental chemistry. The computational effort at Pacific Northwest Laboratory is supported by both the Office of Basic Energy Sciences and the High Performance Computing Program.

Successful Experimental Run Completed at the Stanford Synchrotron Radiation Laboratory

The Stanford Synchrotron Radiation Laboratory, operated by the Office of Basic Energy Sciences, has just completed a very successful 7 month run in which 89.5% of the scheduled beam was delivered to users. During the last week of the run there was a record-breaking 98.5% beam delivery to users. The 26 experimental stations accommodated 325 separate experiments from 136 individual spokespersons representing 50 institutions during this period. The distribution of experiments was 44% from universities, 34% from federal laboratories, 17% from private institutions and 3% involving foreign scientists. There were 550 users of the facility during this period. Significant efforts on studying problems related to nuclear waste remediation were begun, with groups from Los Alamos and Pacific Northwest Laboratories running on adjacent stations the last two weeks.

Basic Research "Spins Off" Equipment for Semiconductor Materials Growth

Sandia National Laboratories/Albuquerque has recently shipped a scaled-up rotating-disk reactor (RDR) to SEMATECH for use in their chemical vapor deposition (CVD) process development programs. The technology behind the Sandia RDR was originally developed as part of an Office of Basic Energy Sciences/Materials Sciences sponsored program in CVD Science. CVD is a critical component in the processing of most semiconductor materials, as well as a host of other high-tech materials syntheses. In studying the complex chemistry of CVD processes, it was often found that fluid-flow conditions in existing commercial CVD reactors made it nearly impossible to develop accurate models of the chemically reacting flow leading to materials growth. The concept of the rotating-disk reactor was thus pursued (starting in 1987) as a way to greatly simplify studies of the fundamental chemistry by recasting the fluid mechanics side of the problem into a well defined geometry that was computationally attractive.

In large part due to Sandia's demonstrated expertise in modeling of CVD processes, the Materials Sciences CVD Science program has led to several follow-on programs funded by the Department of Energy/Defense Programs and Defense Advanced Research Projects Agency to work with industry in advancing the development of CVD reactors through the use of scientifically based models of the chemical processes. One such program with SEMATECH involved using the numerical models of the Materials Sciences developed 2-inch diameter research RDR to design a scaled-up 6-inch diameter RDR and demonstrate that growth-rates in the larger reactor could be predicted from the original model. After successfully demonstrating the latter, Sandia has now shipped (the last week of August 1992) the larger scale RDR to SEMATECH where they will use it for further research on reactor and process design and optimization.

While the delivery of an advanced design reactor to SEMATECH is a noteworthy event, even more significant is that it represents a growing acceptance by industry that basic scientific research can lead to real improvements in product design. Up to now, semiconductor process reactors have been almost exclusively designed via "cut and try" methods. As a consequence, product improvement is incremental, costly, and often risky. In contrast, numerical models based on a scientific understanding of the underlying physics and chemistry allow intelligent design of CVD processing equipment which can lead to superior equipment performance and reduce development costs. In the long run, these lower costs and improved performance mean a more competitive industry, which will benefit the U.S. economy.

Productive Partnership Fostered with Electric Power Research Institute

Dr. Robert Gottschall from the Office of Basic Energy Sciences/Division of Materials Sciences presented a seminar and discussed programmatic issues and cooperation at the Electric Power Research Institute in Palo Alto, California, on June 25, 1993. The Electric Power Research Institute and the Office of Basic Energy Sciences have many common scientific and technical priority needs, and numerous university and national laboratory investigators have support funding from both organizations on complementary, but non-overlapping, research tasks. The Electric Power Research Institute staff have been regular participants in the Office of Basic Energy Sciences Contractor meetings on aqueous corrosion and welding, and the Division of Materials Sciences and the Electric Power Research Institute have jointly sponsored two Research Assistance Task Forces (on weld modeling and predicting fracture behavior of welds) during the past year.

The Electric Power Research Institute presently has some Cooperative Research and Development Agreements with the Department of Energy. However, the discussions between Dr. Gottschall and the Electric Power Research Institute staff focussed on future common research needs and opportunities and programmatic interfacing in the areas of non-destructive evaluation, gaseous corrosion, aqueous corrosion, welding and critical materials issues in steam, fossil- fired, boiling water nuclear reactor, and solar energy conversion systems. The visit to the Electric Power Research Institute was part of a standing series of exchange visits between the Electric Power Research Institute and the Office of Basic Energy Sciences staff.

Atlas of Spectral Data Helps Analysis of Environmental Pollutants

Inductively coupled plasma atomic emission spectroscopy, which resulted from Office of Basic Energy Sciences/Chemical Sciences Division support, has become one of the premier techniques in the world for the elemental analysis of metals. As a result, a need rapidly evolved for a standardized data base of elemental spectral line information for inductively coupled plasma atomic emission spectroscopy. This need is being met through the publication of the *Ames Laboratory ICP Atlas* of atomic spectral lines. The growing use of inductively coupled plasma atomic emission spectroscopy for the environmental analysis of pollution sources, waste management, and characterization and remediation of hazardous waste sites is driving the necessity for this type of information, which helps in the qualitative and quantitative interpretation of the spectra. Initial inductively coupled plasma atomic emission spectroscopy research funded by the Division of Chemical Sciences in the late 1960's and early 1970's was aimed at the fundamental understanding of this newly developed technique. The Atlas is predicated on this initial research of Chemical Sciences investigator Velmer Fassel and carried out by his colleagues Royce Winge and David Eckels at Ames Laboratory. This Atlas represents the out-growth of basic research supported through Basic Energy Sciences and is a good example of technology transfer between Chemical Sciences and the outside technology community.

Joint Workshop Focuses on Usefulness of Laser Techniques

The biennial joint meeting of OHER and OBES research investigators who use a variety of laser techniques in their research endeavors was held in Sante Fe, New Mexico, on October 19-21, 1992. These meetings have been organized informally over the past fifteen years. ER was represented by Roland F. Hirsch from OHER and Clement R. Yonker from OBES. This conference provides an important forum for the reporting of research results and the cross-fertilization of ideas between OHER and OBES investigators in the expanding use of lasers for chemical characterization. Of particular note was the invited talk by W. E. Moerner of the IBM Almaden Research Laboratory in which he described the optical probing of single molecules in solids. Another subject of importance addressed the advances in chemical imaging on a submicron scale with potential applications ranging from cellular biology to materials science.

Workshop Held on Application of Positron Spectroscopy in Materials Sciences

A workshop on "The Application of Positron Spectroscopy in Materials Science" sponsored by the Office of Basic Energy Sciences/Division of Materials Sciences (OBES/DMS), was held in Rancho Mirage, California, September 9-11, 1992. The purpose was to identify new and emerging research needs and opportunities. The chairpersons were Dr. Yok Chen (on part-time assignment to Materials Sciences from Oak Ridge National Laboratory) and Dr. Lester D. Hulett (from Oak Ridge National Laboratory). The keynote lecture was delivered by Allen P. Mills of AT&T. The 29 participants were from industry (6), DOE laboratories (7), universities (9), DOE (2 - Dr. Chen and one observer from Conservation) and abroad (5). Recent and anticipated future advances in positron sources, beams and associated facilities and the advent of monoenergetic beams now permit a new level of characterization of defect, electronic, surface and interfacial structure. These advances will also permit (1) the characterization of certain dynamic properties on previously unattainable scales of real time, and (2) achievement of spatial resolution ranging from the millimeter to the nanometer scale. The purpose of the written proceedings of this workshop is to broadly disseminate the new and emerging research needs and opportunities that were identified, and these proceedings are being submitted to a refereed scientific journal for publication so as to enhance this dissemination.

Dr. Dragoo Presents Seminar at Corning

Dr. Alan L. Dragoo of the Office of Basic Energy Sciences/Materials Sciences Division visited Corning to present a seminar to the research staff and to tour the research facility on September 14, 1993. This visit is part of Materials Sciences' efforts to develop a greater awareness of materials research issues and activities in the private sector and to inform companies of the materials research program funded through the Office of Basic Energy Sciences. Glass science and technology, including heat resistant glasses, machinable glass-ceramics and optical fibers, have been at the center of Corning's research and development as well as its commercial activity. The Division of Materials Sciences, through its Metallurgy and Ceramics Branch, has supported work on the strength and fracture of glass and fundamental studies of glass structure. Materials Sciences considers that it is important for its basic research program to provide improved understanding of material properties and phenomena which meet the needs and issues of industry.

Licensing Agreement for Superconductor Precursor Process Builds on Capabilities Established by Basic Research

A license agreement (May 12, 1993), between Superconductive Components, Inc., and Martin Marietta Energy Systems, Inc., managing contractor for the Oak Ridge National Laboratory, was announced in a press release. With funding from the Department of Energy's Office of Energy Management/Superconducting Technology Program, researchers at Oak Ridge National Laboratory developed an improved process to prepare highly uniform, chemically homogeneous, fine-grained powders of mixed-oxide high transition-temperature superconductors that contain lead as one of the metallic components. The key improvement, which Superconductive Components, Inc., plans to scale up and commercialize, lies in development of aerosol pyrolysis conditions that avoid the loss of volatile lead components that typically occurs during powder preparation.

One of the Oak Ridge National Laboratory researchers, Jorulf Brynestad of the Chemistry Division, has also been partly funded by the Office of Basic Energy Sciences/Division of Materials Sciences to carry out research on fundamental aspects of synthesis and characterization of high transition-temperature superconductors ever since the initial interest in this topic arose. Particular emphasis is placed on methods to control exact chemical compositions and phase relationships during preparation of these complex multi-component materials. Several of the oxide compositions of current interest contain metals, such as thallium, lead, and mercury, that tend to escape as volatile species at the elevated temperatures required for synthesis. Such loss results in non-homogeneous products of non-optimum composition and hence in seriously degraded performance properties. Defining scientific bases to counteract this phenomenon has been central to the work supported by the Office of Basic Energy Sciences. The invention and license agreement represents a specific embodiment of such generic undergirding research knowledge and capabilities.

Innovative Oil-Spill Cleanup Method Receives Publicity

An article on the novel oil cleanup method developed by Professor Adam Heller, who was supported by the Office of Basic Energy Sciences/Division of Advanced Energy Projects, appeared in the Sunday, August 15, 1993, issue of the *New York Times*. On August 19, 1993, the Oil Pollution Act of 1990 went into effect. This law, passed in response to the Exxon Valdez oil spill, mandates that companies involved in storing and transporting oil have standby plans for cleaning up oil spills on land or in water. This law creates opportunities for new cleanup technologies and give impetus to an industry that is already a $1 billion-a-year business.

Professor Heller's approach utilizes tiny hollow glass beads covered with titanium dioxide; when these beads are sprinkled on an oil spill, the oil coats them and the titanium dioxide acts as a photocatalyst, allowing sunlight to reduce the oil to carbon dioxide and water. The residue is nontoxic, consisting of sand-like particles that float and can be skimmed up or allowed to float ashore. In the article it is pointed out that this concept is one of two promising new approaches to oil cleanup.

Professor Heller has formed a company, Heller Environmental Inc., to exploit the new technology. The article states that Texas is interested in using this process for cleanup of oil spills off the Gulf Coast, which would be the first field test of the beads. The research to develop Professor Heller's process was supported by a grant from the Office of Basic Energy Sciences/Division of Advanced Energy Projects.

Lawrence Berkeley Laboratory Receives Unrestricted Industrial Gift for Tribiology Research

Komag, Inc., a small business located in Milpitas, California, which manufactures magnetic disks, has sent a $30,000 check to the University of California that represents an unrestricted gift to the Center for Advanced Materials at the Lawrence Berkeley Laboratory. The gift will be used in an Office of Basic Energy Sciences/Materials Sciences Division-sponsored program in the area of amorphous carbon films. As part of this research, the structure of carbon films will be studied by surface analysis of elemental composition and in depth profiles of sputtered fragments ejected by ion impact.

The Center for Advanced Materials annually receives about ten unrestricted gifts from industrial companies to perform basic research in areas of interest to United States industry.

General Motors Endorses Materials Sciences Research in Superplastic Forming Alloys

As part of the review of the Laboratory Field Task Proposals, the Division of Materials Sciences approved a new effort at Pacific Northwest Laboratory entitled "Interfacial Dynamics During Heterogeneous Deformation." According to a letter to Dr. Iran Thomas from Dr. Richard W. Marczewski of the General Motors Research and Development Technology Leveraging Center, the research "would complement General Motor's research and development efforts in superplastic forming by developing a mechanistic understanding of interfacial behavior during high-rate superplastic deformation." Dr. Marczewski further noted that "We feel that the fundamental research addressed in this proposal would provide a much needed basis for the design and development of superplastic forming alloys and processing methods which have broad commercial applications ... In summary, General Motors believes that basic materials research directed at understanding superplastic deformation mechanisms for aluminum alloys would complement General Motor's objectives in applying this technology to lightweight vehicles." This new program joins the other ongoing efforts funded by Materials Sciences in the area of plastic deformation behavior of metals and alloys.

Industrial Activities Continue at the Materials Preparation Center, Ames Laboratory

The Materials Referral System and Hotline at the Ames Laboratory's Materials Preparation Center received 270 request for help in locating materials preparation and characterization services during the period July 1-December 31, 1992. The most frequent category of user of this service is the private industrial sector, which placed about 55 percent of the inquiries. The second most frequent user, the university category, placed about 31 percent of the inquiries. The remainder was divided among the Department of Energy laboratories and non-Department of Energy government laboratories or agencies. The Materials Preparation Center also publishes *The High-T_c Update* which continues to serve the needs of the laboratory-university-industrial superconductivity community.

The gross sales to outside organizations of materials and services of the Materials Preparation Center over this six-month period came to $164,951.80 based on 75 sales. The percentage analysis of outside orders was 34 percent private sector, 26 percent universities, 23 percent Department of Energy and other government laboratories, and 17 percent foreign. Recent activities include further interactions with General Electric Medical Systems to prepare a specialized braze alloy for medical diagnostic application, the preparation of gadolinium compounds for new magnetic refrigeration applications for Astronautics Corporation of America, the preparation and analysis of lanthanum-tin compound for hydrogen refrigeration studies for Aerojet Electronic Systems Division of Aerojet General, and interactions with the National High Magnetic Field Laboratory concerning the preparation of higher strength wire of a refractory copper alloy.

In addition to providing materials for specific research projects at the Ames Laboratory, the Ames Materials Processing Center actively and effectively assists in the transfer of its unique technologies . Some of the industrial laboratories which obtained services from the MPC during the past year include AT&T Bell Laboratories; Battelle Memorial Institute; Bausch and Lomb; Bellcore; Bendix Corporation; Boulder Scientific; Edge Technologies; EPRI; Eveready Battery Company; Failure Analysis Associates; G.E. Medical Systems; General Electric Company; GM Research Center; GM Research Laboratory; GTE Laboratories, Waltham, MA; IBM Almaden Research Center; IBM Research Center; IBM Research Division, T. J. Watson Research Center; IGC; II-VI Inc.; Integrated Chemical Sensor Corporation; Intersonics Inc.; Jet Propulsion Laboratory; Metallamics; MicroBeam Inc.; Pratt and Whitney Aircraft; Research Chemicals; Rocketdyne Division of Rockwell International; Sausville Chemical Co.; Specialty Materials Laboratory; Supercon, Inc.; TOSHOH SMD, Inc.; Tracer Technologies; Universal Energy Systems; Universal Energy Systems. Government laboratories receiving help from the MPC included six DOE laboratories, NASA Langley Research Center, National Institute of Standards and Technology, Naval Research Laboratory, and the Naval Surface Warfare Center. Twenty-six universities also were helped by the MPC.

The MPC had a exhibit booth at the Materials Research Society meeting in Boston on November 30 - December 4, 1992. It included samples of commercially unavailable pure rare-earth oxides and pure rare-earth binary alloys, intermetallic and II-VI compounds, and a brochure. This meeting attracted 4000 registrants.

The Materials Referral System and Hotline (MRSH) at the Ames Laboratory's Materials Preparation Center (MPC) received 340 requests for help in locating materials preparation and characterization services during the period January 1 - June 30, 1992. This number is the same as that for the previous 6-month reporting period.

The most frequent category of user of this service is the private industrial sector, which placed about 60 percent of the inquiries. The second most frequent university category placed 20 percent of the inquiries. Approximately 15 percent of the inquiries come from DOE laboratories and another 5 percent from non-DOE government laboratories or agencies.

The gross sales receipts to outside organizations of the materials and services of the MPC over this 6-month period came to $128,458.51, which is less than that for the previous 6-month reporting period, partially as a consequence of the allocation of effort to Tiger Team preparations. The number of MPC interactions during this 6-month period was 73, whereas it was 71 for the previous 6-month period. Interactions over the past 2 years with Dr. T. Tiearney of General Electric Medical Systems have lead to an on-going effort to prepare a specialized braze alloy for medical instrument application. Efforts have been initiated to prepare a copper-niobium alloy for Los Alamos National Laboratory as part of a materials development program for the National High Magnetic Field Laboratory at the University of Florida.

Fundamental Separations Research Impacts Commercial Water Quality Analysis

A newly commercialized instrument to significantly advance water quality analysis is based on Office of Basic Energy Sciences-funded research. This instrument, called ExCell (from extraction cell) is marketed by the ABC (Analytical BioChemical) Laboratory, and provides for faster, more efficient and accurate analyses of water quality. It was derived from an emulsion phase contactor which was developed in a basic research project at the Oak Ridge National Laboratory. This contactor is the result of Chemical Sciences-supported basic separations research and developed with support from the Division of Advanced Energy Projects. The ExCell instrument was featured in a popular exhibit at the March, 1993, meeting of the Pittsburgh Conference on Analytical Chemistry in Atlanta.

Basic Research on Control of Coating Processes Improves Office Supply Product

Coating processes are critical to manufacturing of magnetic and optical memory storage media, adhesives, and paper products. The usual limited control of the flow of the coating material onto a moving tape or other substrate materials has caused imperfect products and costly waste.

Studies supported by the Office of Basic Energy Sciences/Engineering Research Program at California Institute of Technology have addressed the general problem of devising robust process control systems. Such controls are intended to make a given process more efficient and less vulnerable to disruptions, thus reducing unforeseen down-times.

Recently, Professor M. Morari, the Principal Investigator on the project recognized that his work on robust control can be readily used to reject many common disturbances which cause coating non-uniformities in a wide range of industrial coating processes. That has helped a leading manufacturer of office supplies to improve the manufacture of coated paper products, such as gummed labels. As much as 80% reduction of the variance in coating thickness can be achieved, as compared with current control methods. The net result is a more economical production of an improved common product.

Dow Chemical Company has Joined a Collaborative Access Team at the Advanced Photon Source

The Dow Chemical Company has evaluated the Collaborative Access Teams at the Advanced Photon Source and has decided to join with DuPont and Northwestern University in the formation of the Dow Northwestern DuPont - Collaborative Access Team. Dow has made a commitment to support 20 percent of the construction costs of the Dow Northwestern DuPont - Collaborative Access Team beamlines and a similar share of the operating costs for a 10-year period. (Twenty percent of the construction costs represents $1.75 million). Dow has 15 scientists who expect to make use of the Dow Northwestern DuPont - Collaborative Access Team's facilities.

DuPont has already made a similar commitment for 40 percent of the construction and operating costs of the Dow Northwestern DuPont - Collaborative Access Team and Northwestern University has a $2.1 million proposal now being considered by the Division of Materials Sciences.

This is another demonstration of the future usefulness of the Advanced Photon Source foreseen by the United States industry.

Quantum Chemistry Computer Programs Become Generally Available

Ever since the advent of machine computation, computer programs have been written to calculate the structures and energies of molecules. The accuracy, reliability, and therefore usefulness of these programs depend on the complexity of the molecule and its electronic structure but have nevertheless steadily increased over the years and can now be routinely used for a variety of applications. Scientists at Argonne National Laboratory in collaboration with researchers worldwide have been working in recent years on the development of the COLUMBUS Program System, so-called because of the association with discovery and exploration of new territory and because of its origins in Columbus, Ohio from researchers at Ohio State University and Battelle Columbus Laboratories. This system has been developed to characterize in great detail the thermodynamic properties and rates of chemical reactions of small molecular fragments important in combustion. However its usefulness for computer aided design of chemical processes was recognized early on and in the development of the system's component programs, great attention has been paid to their portability, the ability of a program to run on many different machines, and to their accuracy as verified by laboratory experiments. On Columbus Day in 1991, the Columbus Program System was made available to the scientific community in general over the Internet. Since that time, the entire program system has been copied about 150 times and individual component files are being accessed at a rate greater than 50 times a week. Industrial users include DuPont, Allied Signal, Amoco, and United Technologies. The access allows for feedback from the users for future improvements.

Iowa Companies Assistance Program Established at Ames Laboratory

The Iowa Companies Assistance Program has been established with State of Iowa funding to promote interactions with the Iowa industrial community by establishing a technical assistance program through the Institute for Physical Research and Technology/Ames Laboratory's Materials Preparation Center. This program offers services primarily in the field of materials preparation, processing and characterization although all technical areas of the Ames Laboratory and the Institute for Physical Research and Technology centers may become involved. The interaction with Iowa businesses involves preparing custom tailored materials, providing analytical and characterization services and assistance through technical consulting. These services are utilized by the companies to assist in the resolution of commercial manufacturing problems. This program introduces the Iowa business community to the facilities available at the Materials Preparation Center, Institute for Physical Research and Technology centers and the Ames Laboratory and may serve to foster additional, larger industrial interactions.

The Materials Preparation Center offers a wide variety of services which would benefit commercial manufacturing operations. These capabilities include preparation of custom and/or specialty metals and alloys for substitution of current materials or for use in the development of a new product. In addition, characterization services such as analytical techniques for chemical, surface or microstructural analysis will assist in the resolution of quality control issues and improvements in overall manufacturing operations. All interactions, materials and services will remain confidential. Implementation of this technical assistance program creates a significant resource for the Iowa business community and assist in their ability to compete in an increasingly global marketplace.

Strong Industrial Collaborations Continue at Brookhaven National Laboratory

Four recent written testimonials have been received concerning industrial interactions with the Materials Sciences program at Brookhaven National Laboratory.

S. R. Prescott of W. P. Grace and Company, referring to collaborative work between his company and H. Issacs/A. Davenport, noted: "The initial results of this collaborative work have been quite encouraging and have provided us with new insights on the mechanisms of corrosion inhibition...We hope to continue our collaboration studies with Brookhaven National Laboratory...."

F. Namavar of Spire Corporation noted: "the invaluable efforts in our collaboration over the past several years" with S. Heald regarding extended edge X-ray absorption fine structure analysis of thin films and interfaces in semiconductor systems.

M. Kendig of the Rockwell International Science Center acknowledges their informal collaboration with A. Davenport and H. Isaacs "to investigate an important problem faced by the aerospace industry, specifically how to provide corrosion protection to aluminum alloys without using environmentally hazardous hexavalent chromium compounds." Kendig goes on, "I sincerely appreciate the unique resources available at Brookhaven National Laboratory and the freedom of your staff for informal collaborations such as ours."

J. Sinclair of AT&T, writing about collaborative work with A. Davenport and H. Issacs, noted the intent "...to understand the chemical reactions that occur at metal/polymer interfaces so that process chemistry and conditions can be optimized to produce high quality interfaces. These interfaces are very important in the packaging of electronics, from integrated circuits and multi-chip modules to printed circuit board assemblies" and went on to cite contributions by Davenport and Isaacs at several levels and "encourage Brookhaven National Laboratory to continue to collaborate with American companies."

"Modeling for Welding Science" Research Assistance Task Force

A number of areas for multidisciplinary collaborations were identified in a Research Assistance Task Force (RATF) Workshop on "Modeling for Welding Science" held March 17-19, 1993. This RATF was co-sponsored by the Division of Materials Sciences, Basic Energy Sciences, and the Electric Power Research Institute. The organizers were Thomas Zacharia and John Vitek, Oak Ridge National Laboratory, and R. "Vis" Viswanathan, Electric Power Research Institute. There were 26 participants with 4 from industry, 14 from universities, 6 from national laboratories, and one each from the Department of Energy and the National Institute of Standards and Technology. The international welding modeling community was represented with participants from the United States and 5 other countries.

The goals of the workshop were to evaluate the current status and future directions of weld modeling and to promote interactions among the various weld modeling activities to achieve an integrated capacity to model the entire welding process. The four major areas addressed were: (1) heat and fluid flow, (2) heat source/metal interaction, (3) weld solidification microstructure, and (4) phase transformations. The workshop identified possible mechanisms to develop long-term multidisciplinary collaborations including the establishment of databases, a repository for models subroutines, and software packages needed to establish effective technology transfer within the welding community. The first draft of the report of the findings is completed. When final, the report will be published in *Modeling and Simulation in Materials Science and Engineering*, a journal sponsored by the Institute of Physics. Joseph B. Darby represented the Division of Materials Sciences at the workshop.

Collaborations of Office of Basic Energy Sciences Researchers with Amoco

Dr. Frank Y. Fradin, from Argonne National Laboratory, sent a copy of a letter to him from Dr. Theo H. Fleisch, Director of Natural Gas Research at Amoco Corporation. Dr. Fleisch highlighted three areas: fluid cracking catalysts, nucleation and crystal growth of zeolites from aluminosilicate gels, and novel molecular sieve materials for methane activation and conversion of natural gas to higher hydrocarbons. The latter project has evolved into a cooperative research and development agreement between Amoco and Argonne National Laboratory. This project was reviewed by the Office of Program Analysis and received a low mark because of the lack of actual catalysis work. It is focused on synthesis at Argonne, but the reviewers did not consider the interactions with other programs. The letter also points out the value of the Stanford Synchrotron Radiation Laboratory, the Intense Pulsed Neutron Source, and other research at Argonne that is of considerable long-term interest to Amoco.

Twelve Predoctoral Fellowship Awards Made in Integrated Manufacturing

On March 7-9, 1993, a panel consisting of leading researchers in the field of manufacturing drawn from industry and universities chose twelve applications for the award of 3-year Department of Energy-National Academy of Engineering-National Research Council fellowships in integrated manufacturing. Of the 225 preliminary applications, there were 145 final applications received. The recipients of the fellowship will pursue their Ph.D. studies at Georgia Institute of Technology, Massachusetts Institute of Technology, Purdue University, University of Michigan, University of Illinois, Oregon State University, Pennsylvania State University, Carnegie Melon University and University of Washington. They will investigate manufacturing process control problems, instrumentation, application of computers to the integration of the design and manufacture of discrete parts, and man/machine interfaces. A list of the fellows and their proposed research topics is available from the Office of Basic Energy Sciences/Engineering and Geosciences Division.

Atomic Force Microscopy (AFM) Illuminates Surface Features of Advanced Polymers

A research group at the Center for Advanced Materials at Lawrence Berkeley Laboratory (LBL) has obtained images of the industrially and medically important polymer UHMWPE (ultra-high molecular weight polyethylene) using the AFM.

UHMWPE is used extensively for medical implants. Its wear attributes, however, have not been fully characterized. These new results demonstrate the likelihood that the AFM can provide information about the surface properties of the polymer and, therefore, the effect of wear on those properties. Preliminary results have suggested, for example, that light acid etching (a test of physiological effects on long-term implants) results in significant changes in the AFM image, although a more complete explanation remains to be determined.

This work involves a collaboration of scientists at LBL, at DuPont, and at a company, Diatome International, in Biel, Switzerland. The key to the success of the study was sample preparation, which involved diamond-knife cyromicrotoming at -170°C, achieved in collaboration with H. Gnaegi, Diatome International, Biel, Switzerland. The images obtained were marked by light striations representing features up to 500A about the base plane. Comparison with transmission electron micrographs obtained by Barbara Wood at DuPont suggests that these regions represent the crystalline phase standing out from the amorphous regions of the polymer.

Air Conditioning Industry Using Data from the Instrumentation Program

Under the direction of Dr. Richard Kayser, Head of the Thermophysics Division at the National Institute of Standards and Technology (NIST), more than a dozen new state-of-the-art instruments have been developed and put into routine operation for measuring the thermophysical properties of fluids important to the chemical and energy-related industries. Critically needed measurements for various energy-related fluids have led to the development of models and a computer package called REFPROP which, to date, has been purchased by more than 200 users. The Alternative Refrigerants Evaluation Program of the Air Conditioning and Refrigeration Institute has adopted REFPROP as its source of thermodynamic properties data. The goal is to provide the air conditioning and refrigeration industries with properties data they need to replace ozone-depleting CFC's and HCFC's with environmentally acceptable alternatives. As an example, comprehensive data has been obtained for the refrigerant R-134a (1, 1, 1, 2-tetrafluoroethane), which is a promising replacement for R-12 (diflourodichoromethane), for use in automobile air conditioners and home refrigerators and freezers. The Engineering Research Program of the BES/Division of Engineering and Geosciences has provided support to NIST for the development of the critical instrumentation.

Ultrasensitive High-Temperature Superconductor Magnetometer Fabricated

A Lawrence Berkeley Laboratory research group under the direction of John Clarke and supported by the Office of Basic Energy Sciences/Division of Materials Sciences has fabricated a novel, ultrasensitive magnetometer based on a Superconducting Quantum Interference Device using high transition temperature superconductors and operating in liquid nitrogen at 77 Kelvin. This device has achieved an extraordinary magnetic field resolution at frequencies extending down to about 1 Hertz. This resolution, for the first time, meets the needs of applications such as geophysical surveying and routine magnetocardiology, and represents the best performance yet reported for any magnetometer operated at 77 Kelvin.

The magnetometer is made from a patterned thin film of a high-temperature superconductor. The film is structured to form two Josephson junctions where it crosses the 24 degree grain boundary of the substrate. The magnetic field sensitivity is enhanced by depositing, in the same process, a pick-up loop that is connected to the body of the Superconducting Quantum Interference Device. A magnetic field applied to the pick-up loop injects current directly into the Superconducting Quantum Interference Device. When in use, the Superconducting Quantum Interference Device is immersed in liquid nitrogen and operated in a flux-locked loop.

This "direct-coupled magnetometer" is simple to manufacture and the process has a high yield. The technology has already been transferred to Conductus, Incorporated. A 3-axis magnetometer, containing three such devices and intended for geophysical applications, will be field tested this summer. Immersed in a novel liquid nitrogen dewar, designed in collaboration with Conductus and Advanced Cryogenic Systems, the system is expected to be the first such device with an operating time of several months without replenishment of the cryogen.

Cooperative Research and Development Agreements (CRADAs)

At the beginning of Fiscal Year 1994, over 500 CRADAs have been signed between Department of Energy national laboratories and U.S. industry. A disproportionately large fraction of DOE CRADAs are either directly funded by Basic Energy Sciences (BES) or stem from BES-supported work at the laboratories. Presented below are seventeen recent examples of such CRADAs.

Computer Simulation and Modeling of Polymers Leads to CRADA with Hoechst Celanese Corporation

In a feature article and cover story in the June 1993 issue of *Trends in Polymer Science*, a new journal that provides authoritative overviews of recent advances, B.G. Sumpter, D.W. Noid, and B. Wunderlich of the Oak Ridge National

Laboratory discuss the state-of-the-art in computer simulations of macromolecular systems (for example, polymers). Recent advances in computer simulation techniques as well as in computer hardware, such as massively parallel computers, have provided the necessary tools for performing larger and more accurate computations. It is now possible to carry out detailed simulations of the microscopic motions of macromolecules containing as many as 100,000 atoms. Such computer simulations provide much of the data needed to link the microscopic description of the atomic motion with the experimentally observed macroscopic changes. The article describes results from computations using novel techniques, such as high-resolution spectral estimators, neural networks, and efficient molecular dynamic methods that have been developed at Oak Ridge with Office of Basic Energy Sciences/ Division of Materials Sciences support. This work led to a Cooperative Research and Development Agreement between Oak Ridge National Laboratory and Hoechst Celanese Corporation, a major international polymers company, entitled "Atomistic Simulation of Materials: A Neural Network Approach." This agreement based on the Materials Sciences research was funded by Defense Programs and signed in September 1992.

Basic Science of Metals Provides Basis for Los Alamos-General Motors CRADA

On April 12, 1993, a Cooperative Research and Development Agreement was signed between Los Alamos National Laboratory and General Motors Research Laboratory to apply results of the Division of Materials Sciences Metallurgy Program at Los Alamos to the process of metal cutting.

Rapid metal cutting is a very important area for U.S. manufacturing. U.S. exports of metal working machinery totaled $1.6 billion dollars in 1987. However, the U.S. share of the world market has declined from fifty percent in recent years to ten percent in 1990. Metal cutting is a very important and costly step in many manufacturing processes. Tool wear, surface finish, chip size, and removal are all extremely important issues. By addressing these issues using computer simulation, prototyping costs and large amounts of time can be saved. Metal cutting is inherently a very high strain rate process. High temperatures, on the order of hundreds of degrees celsius, are generated by the high strain rates. In addition, most materials shaped by metal cutting have a preferred texture and, hence, their properties are anisotropic with respect to stressing direction and stress state. The Mechanical Properties Program at Los Alamos, which is supported by the Office of Basic Energy Sciences/Division of Materials Sciences, has developed advanced constitutive relations - i.e., physical relationships between properties of the material such as stress, strain, temperature, grain size and texture. Other researchers at Los Alamos, working under support form Defense Programs, have implemented these constitutive relations into explicit Finite Element Model codes to model strain and temperature contours in worked materials. The modeling and simulation tools that Los Alamos is developing with General Motors Research Laboratory have the potential to produce significant savings.

Basic Studies of Solvent Extraction Part of CRADA on Aerial Spraying

A consortium of 27 companies called the Spray Drift Task Force (SDTF) led by DuPont and having interest in the fundamentals of aerial spraying of crops has entered into a CRADA with a long-term Office of Basic Energy Sciences/Chemical Sciences Division research project at the Oak Ridge National Laboratory. The research project under the leadership of Dr. Osman Basaran focuses on the fundamental principles of solvent extraction and has developed a method for the measurement of the dynamic surface tension of droplets. The method is cable of determining tension as a function of time on the millisecond scale and its generality has been demonstrated by making measurements on droplets having diversely different chemical content. This expertise is of critical interest to the SDTF as it will guide the design of spraying equipment and nozzle configuration and provide information on the proper chemical content of the spray solution, amount and types of surfactants, and speed of droplet formation, among other variables.

Lawrence Berkeley Laboratory and International Business Machines Signs a CRADA on Computer Hard Disks

A Cooperative Research and Development Agreement was signed by Lawrence Berkeley Laboratory and the International Business Machines Corporation on January 15, 1993, for the preparation and characterization of novel lubricated hard carbon protective coatings for computer hard disks.

The project involves the detailed, atomic level surface characterization of sputtered hard carbon films produced by International Business Machines. The goal is to obtain precise knowledge of the chemical composition of the surfaces of the films by using a variety of electron spectroscopies to provide correlations between surface chemical composition and the conditions under which the film was produced.

Researchers will also study the surface chemistry of the hard carbon films to understand the nature of the bonding of lubricant molecules to carbon surfaces, with a view towards modifying processing conditions to optimize the adherence of the film. Finally, researchers will study the mechanical properties of the hard carbon films and the lubricated surfaces in an attempt to correlate the atomic level surface composition and structure of the hard carbon films to hardness, friction, and wear.

The collaboration is based on Lawrence Berkeley Laboratory facilities and expertise developed over the past 25 years as part of a fundamental research program in surface science supported by the Office of Basic Energy Sciences/Division of Materials Sciences. In the course of that program, the Lawrence Berkeley Laboratory group has built a state-of-the-art surface analysis facility that includes X-ray Photoelectron Spectroscopy, Auger Electron Spectroscopy, Scanning Tunneling Microscopy, Atomic Force Microscopy, and Secondary Ion Mass Spectroscopy. The group has extensive experience in studies of the properties of thin films, having published studies of zirconium oxide, silicon carbide and other related materials, including structural analysis of coatings to which lubricants have been bound. The knowledge and the associated techniques will be easily adapted to the specific systems of interest to the International Business Machines.

Development of Experimental Physics and Industrial Control System Subject of CRADA

The Advanced Photon Source at Argonne National Laboratory, with support from the Division of Materials Sciences in cooperation with the Los Alamos National Laboratory, has developed several additional capabilities and made significant improvements to the Experimental Physics and Industrial Control System software while maintaining complete compatibility with existing software. This control system may soon find application in industrial as well as other Department of Energy laboratory's controls applications at the Department of Energy labs. This system has been developed to control the injection of positron beams into the Advanced Photon Source Storage Ring.

As Argonne and Los Alamos added new and compatible tools and capabilities, it became apparent that the product would be commercially attractive. Los Alamos has proceeded with both a Cooperative Research and Development Agreement and a licensing process, and will soon issue licenses to two industrial companies. The Los Alamos group did the original development work on the system under a Department of Defense contract. The two groups now work together on design specifications, design reviews, and testing. The system is being designed with flexibility in mind while at the same time using state-of-the-art components. Standards are being employed wherever possible to protect the initial investment in components and to keep the hardware vendor-independent. The software is based on a set of compatible "tools" to enable the addition of new capabilities in the future.

Two CRADAs at Los Alamos National Laboratory

Two new Cooperative Research and Development Agreements, originating from research supported at Los Alamos National Laboratory by the Office of Basic Energy Sciences, Division of Materials Sciences, have been initiated. One entitled, "Modeling and Simulation of Electronic and Photonic Devices: Polymers," signed on

September 10, 1992, involves the Hewlett-Packard High Speed Devices Laboratory and is aimed at potential display and optical interconnect applications. The other, with Radiant Technologies, Inc., signed on August 27, 1992, is entitled, "Conductive Oxide Electrodes for Ferroelectric Memory Development," and related to possible thin film electrodes and ferroelectric devices. Both are funded under the Technology Transfer Initiative.

Electro-Optical Properties of Nanocrystals are Being Explored in CRADA

The Lawrence Berkeley Laboratory signed a Cooperative Research and Development Agreement with Motorola Inc. on December 17, 1992, to use new materials formed from nanocrystal semiconductor particles to develop a new generation of electro-optical devices. This joint project between Lawrence Berkeley Laboratory and Motorola would transfer the Department of Energy's advanced material research to develop a next generation of devices that would require low voltage and would not depend on current technology.

Lawrence Berkeley Laboratory will fabricate the nanocrystals and will investigate their electro-optical properties. This includes stimulating photon emission in free crystals and in those bound to metal surfaces. Various methods of binding the nanocrystal particles to conducting metals will also be investigated. Motorola Incorporated also plans to measure the electro-optical properties of the novel nanocrystal structures. Motorola will emphasize analysis of structures developed on this project which indicate commercial transfer potential. In addition to performing experiments, Motorola's plans include performing a full analysis of activities necessary to commercialize the Department of Energy's technology.

The fundamental research of Paul Alvisatos in the preparation, production and characterization of semiconductor nanocrystals was supported, first by Laboratory Directed Research and Development funds and then by the Office of Basic Energy Sciences/Division of Materials Sciences.

Fundamental Research on Intelligent Machines Underpins CRADA with AMTEX

The Oak Ridge National Laboratory-Center for Engineering Science Advanced Research program is represented on an interlaboratory team preparing a proposal to the AMTEX (U.S. textile industry trade group) Steering Committee. Oak Ridge National Laboratory plans to support the necessary developments in the area of information processing, data analysis, communications and modeling for the textile industry. The prospect for significant contribution by the Center for Engineering Science Advanced Research in the realm of data fusion, pattern recognition, and heterogeneous computing environments rests on the long-term basic research supported by Office of Basic Energy Sciences Engineering Research Program. That fundamental work aims at establishing the scientific infra-structure for enabling technologies in the field of energy related intelligent systems.

Lawrence Berkeley Laboratory and Glycomed Sign CRADA for Biocompatible Materials

Lawrence Berkeley Laboratory signed a Cooperative Research and Development Agreement with Glycomed, Inc., on February 26, 1993, to collaborate on the design of new biocompatible materials. Among the targeted materials are surface coatings for vehicles in drug delivery systems that would be based on the adhesive properties of surface features of biological molecules.

The project involves the use of a new nanoparticle technology developed at Lawrence Berkeley Laboratory to construct glycoconjugate (sugar/amino acid copolymers) 'libraries' containing a vast number of similar but distinctly different molecules. The libraries will be screened to identify those molecules in them that mimic the oligo- and polysaccharide polymers that have been shown to play a major role in bio-adhesive events, including those implicated in a variety of diseases.

As a part of the Cooperative Research and Development Agreement, Lawrence Berkeley Laboratory will construct the glycoconjugate libraries on the nanoparticles and Glycomed will study the activity of the materials in the libraries. The groups will then collaborate on modifying the design of the best material to optimize activity for drug delivery.

Polymeric materials produced will be marketed by Glycomed as anti-inflammatory agents. Further, the understanding of bioadhesion gained through this industry-lab cooperation may lead to the development of a new class of biocompatible materials for broad use in human implant devices.

Basic research supported over the past 3 years by the Division of Materials Sciences, Basic Energy Sciences, has enabled researcher Mark Bednarski from the Center for Advanced Materials of the Materials Sciences Division to successfully synthesize a variety of new bio-materials using combined chemical and enzymatic methods. This Department of Energy-supported basic research on the development of new carbohydrate-based materials and of nanostructures based on lipids form the basis of the nanoparticles and polymers to be used in the construction of molecular libraries.

<u>Research Applicable to Ferroelectric Memory Development is Subject of CRADA</u>

A CRADA resulting from research at Los Alamos National Laboratory (LANL) supported by the Office of Basic Energy Sciences/Materials Sciences Division has been agreed to by LANL and Radiant Technologies, Inc. The original intent of the research was to investigate the possibility of making thin films of high-temperature superconductors. This, in turn, has led to the process of ferroelecric thin film deposition using pulsed excimer laser deposition. Under the terms of the CRADA, thin film ferroelectric structures for memory applications will be developed and fabricated. For the near term, conductive oxide electrodes with a variety of ferroelectric materials will be used to fabricate device structures. The resulting microstructure will be determined (using ion-beam, x-ray, and TEM analysis) and will be related to performance with regard to hysteretic fatigue, which currently limits random access memory applications. The near-term goal of this proposed project is to develop structure-property relationships that can point the way toward achieving stable hysteretic behavior out to 10^{14} cycles. For the longer term, pulsed excimer laser deposition will be used to synthesize and characterize optimal electrode/ferroelectric thin film structures that would yield high-performance devices and be amenable to large-scale production using organometallic chemical vapor deposition (OMCVD). The CRADA will have a duration of 2 years and an investment of $440 K from Radiant Technologies, Inc.

<u>CRADA Signed Between Texas Instruments and Sandia National Laboratories/Albuquerque</u>

A CRADA for joint research on chemical vapor deposition (CVD) was signed on July 21, 1992, between Texas Instruments (TI) and Sandia National Laboratories. The work covered by the Defense Programs funded Advanced Manufacturing Initiative CRADA, "Application of Imaging of Radical Interacting with Surfaces (IRIS) to Semiconductor Processing," is a direct result of a research program in CVD sciences funded by BES/Division of Materials Sciences. The IRIS technique was developed at Sandia National Laboratories, partly with BES funding, to study chemical reactions important to CVD and plasma systems used for materials processing. TI is interested in improving their understanding and models for CVD processes used in the fabrication of microelectronic devices because it will lead to better processes and equipment designs.

The IRIS technique is used to study how gas-phase chemical intermediates formed in CVD or plasma systems react at surfaces during deposition or etching. It combines molecular beam techniques with spatially-resolved laser induced fluorescence and is the only technique available to directly measure radical/surface reactivities. Studies to date have yielded a surprisingly wide range of radical/surface reactivities demonstrating the need for these kinds of measurements. Accumulating a large number of reactivity measurements will allow trends and analogies with gas-phase reactivities to be analyzed. Drs. Pauline Ho and Richard Bus, of Sandia National Laboratories/Albuquerque, and Mr. Dan White and Mr. Allen Bowing, of TI, are the researchers participating in this CRADA.

Basic Research Transferred to Industry in Thermoelectric Materials CRADA

Martin Marietta Energy Systems, Inc. (MMES), on September 30, 1992, entered into a Cooperative Research and Development Agreement (CRADA) with Marlow Industries to develop high-performance thermoelectric materials. Funded through the Department of Energy/Defense Programs Technology Commercialization Initiative, the 3 year CRADA is based on the application and transfer to industry of materials research capabilities developed in BES-supported (Division of Materials Sciences) programs in materials theory and synthesis. Marlow Industries, a small business with a national leadership position in the manufacture of thermoelectric devices, will collaborate with MMES in an interdisciplinary program of materials design and development aimed at significantly increasing the thermoelectric figure of merit.

Principal Investigators Drs. Brian Sales and Gerald Mahan of the Oak Ridge National Laboratory/Solid State Division will work with Marlow Industries and technical contacts at the Oak Ridge Y-12 Plant to improve the performance of thermoelectric devices for solid-state refrigeration. Using detailed computer simulations, the researchers will investigate a wide variety of materials systems including layered structures and Kondo alloys which show particular promise for thermoelectric applications. Based on theoretical guidance from the computer simulations, MMES will synthesize candidate thermoelectric elements for evaluation. The program will benefit from extensive Basic Energy Sciences development of the theory of thermoelectric materials and related materials preparation and characterization techniques.

This project is the initial phase of a program aimed toward the commercial development of thermoelectric devices which can provide economical cooling for detectors, superconducting electronics, refrigerators, and air conditioners. A modest improvement in thermoelectric efficiency would lead to significant advances in cooling systems for detectors and electronics for defense and commercial applications. A factor-of-three improvement would open a market for air conditioning and refrigeration in the tens of billions of dollars and would provide an alternative to CFC-containing compressor-based cooling systems.

CRADA Signed by Brookhaven National Laboratory (BNL) and EG&G to Develop a Commercial Gamma Ray Detector

Researchers James Cumming and Garman Harbottle of BNL and Sheldon Landsberger of the University of Illinois will be working with E.G. and G. ORTEC Corporation (EG&G), a nuclear measurements instrumentation company based in Oak Ridge, Tennessee, under a recently signed CRADA to develop, test, and help bring to marketplace an instrument that measures gamma radiation.

The device, an Anti-Compton Spectrometer, eliminates the unwanted scattering of gamma rays, known as the Compton effect, thereby making more accurate gamma radiation measurements possible. Extremely precise measurement of gamma radiation is necessary to accurately determine environmental radiation hazards from such sources as radon emanating from the soil. Although the Anti-Compton Spectrometer has been used by the scientific community for 25 years, EG&G will be the first to commercially produce a state-of-the-art instrument for distribution to a worldwide market of environmental and research laboratories.

The CRADA is funded by the Office of Energy Research's Technology Transfer Program, and the support for the basic research at BNL leading to the viability of the project came from the Office of Basic Energy Sciences, Division of Chemical Sciences.

Basic Research on Oxides Leads to MgO Crystal Growth CRADA

A Cooperative Research and Development Agreement (CRADA) between Martin Marietta Energy Systems, Inc., (MMES) and Commercial Crystal Laboratories (CCL) of Naples, Florida, has been negotiated in September 1992 for the purpose of developing new techniques for the growth of large single crystals of magnesium oxide (MgO). This CRADA is being funded through the Department of Energy Research Technology Transfer Program and is based on the accomplishments of a long-term fundamental research effort supported by the BES/Division of Materials Sciences. Commercial Crystal Laboratories is a small business that continues to be a principal U.S. supplier of specialty single crystals for use as substrates for the deposition of thin films of high-temperature superconductors and other materials.

Principal investigators, Y. Chen, M. M. Abraham, and L. A. Boatner of the Oak Ridge National Laboratory (ORNL) Solid State Division have assisted CCL in the area of MgO crystal-growth technology, and their prior contributions were recently recognized in letters of commendation from CCL President Michael Urbanik to U.S. Senators Bob Graham, Albert Gore, and James Sasser. Under the terms of the CRADA, ORNL will build on its MgO crystal growth capabilities, which are unique in the Western Hemisphere, and will cooperate with the CCL technical staff in the development of new techniques for increasing both the size and quality of MgO single crystals.

The scientific basis for the CRADA with CCL was established in the course of BES-supported fundamental-properties studies that were initiated in the late 1960s, and that have subsequently evolved in time to encompass a wide range of both basic and applied materials science investigations of high-temperature materials, such as MgO. The present technological interest in single crystals of MgO stems from its emerging importance as a substrate material for the formation of thin film devices incorporating either the yttrium or bismuth-based families of high-temperature superconductors. The only competing MgO crystal growth technology is foreign based—principally in Japan—and CCL represents the only domestic source for this increasingly important high-technology material.

CRADA on Thermoelectric Materials Cooperative Signed with Marlow Industries

Martin Marietta Energy Systems, Inc. (MMES), entered into a CRADA with Marlow Industries on September 30, 1992, to develop high-performance thermoelectric materials. The CRADA is based on the application and transfer to industry of materials research capabilities developed in the BES/Division of Materials Sciences supported programs at ORNL in materials theory and synthesis and is funded through the Department of Energy Defense Programs Technology Commercialization Initiative. Marlow Industries, a small business with a national leadership position in the manufacture of thermoelectric devices, will collaborate with MMES in an interdisciplinary program of materials design and development aimed at increasing significantly the thermoelectric figure of merit. Principal investigators Drs. Brian Sales and Gerald Mahan of the ORNL Solid State Division will work with Marlow Industries and technical contacts at the Oak Ridge Y-12 Plant to significantly improve the performance of thermoelectric devices for solid-state refrigeration.

This project is the initial phase of a program aimed toward the commercial development of thermoelectric devices which can provide economical cooling for detectors, superconducting electronics, refrigerators, and air conditioners. A modest improvement in thermoelectric efficiency would lead to significant advances in cooling systems for detectors and electronics for defense and commercial applications. A factor-of-three improvement would open a market for air conditioning and refrigeration in the tens of billions of dollars and would provide an alternative to CFC-containing compressor-based cooling systems.

Conducting Polymers Subject of CRADA

A basic research program initiated in 1987 by the BES/Materials Sciences Division has resulted in the signing on August 6, 1992, of a CRADA between Brookhaven National Laboratory (BNL) and Moltech Corporation of Stony Brook, New York. The CRADA involves joint work on developing new conducting and redox polymers. Redox polymers make use of an oxidation-reduction process to store charge much like a battery electrode. The CRADA will, among other things, develop high charge density polymer batteries using redox polymers as the electrode and high conductivity polymers as the electrolyte (BNL holds a patent on the highest Lithium-ion conductivity polymer).

BNL will continue its research on the synthesis and characterization of high conductivity polymers and Moltech will use the new materials in making batteries and related components. The products will then be characterized at BNL using some of the laboratory's unique capabilities. Moltech was established in 1988 to develop applications of a number of materials technologies developed under the basic research program at BNL in collaboration with a research group at New York Polytechnic University.

Small Business Innovation Research

The Small Business Innovation Research Program for the Department of Energy is managed out of the BES Division of Advanced Energy Projects.

Small Business Innovative Research (SBIR) Reauthorized

President Bush signed the SBIR Program Reauthorization Act of 1992 on October 28, 1992. The Act makes the following changes in the SBIR program: (1) The program will be extended from October 1, 1993, to October 1, 2000; (2) The SBIR set aside will be increased from 1.25% of extramural R&D in FY 1992 to the following: 1.5% in FY 1993 and 1994, 2.0% in FY 1995 and 1996, and 2.5% in each fiscal year thereafter; (3) Atomic Energy Defense Programs (AEDP) at the DOE solely for weapons activities or for naval reactor programs will be excluded from the SBIR program. In the original SBIR legislation, which went into effect in FY 1983, **all** AEDP were excluded from SBIR. The new Act added about $5 million of AEDP funds to SBIR in FY 1993; (4) With the new features of the Act indicated in (2) and (3) above, the SBIR budget in FY 1993 was about $50 million. (The FY 1992 SBIR budget was $42.6 million); (5) The maximum amount allowable for Phase I awards will be increased from $50,000 to $100,000. The DOE SBIR FY 1993 solicitation will permit a maximum of $75,000 for Phase I awards; (6) The maximum amount allowable for Phase II awards will be increased from $500,000 to $750,000. But the DOE Phase II award limit will remain at $500,000 for FY 1993; and (7) The evaluation process for Phase II grant applications will contain increased emphasis on commercialization prospects.

SBIR Program Completes Phase I Solicitations

For Fiscal Year (FY) 1993, 168 projects received DOE Phase I SBIR awards of about $75,000 each in response to the first of two FY 1993 solicitations. These grants were selected from among the 1,999 applications submitted by small businesses in response to an SBIR solicitation containing 37 technical topics. In addition, the second solicitation containing 8 technical topics covering new DOE SBIR participants, Environmental Restoration and Waste Management and Arms Control and Nonproliferation, drew 510 grant applications. An additional 32 Phase I awards were made on December 28, 1993, from the second solicitation.

SBIR Program Makes Phase II Award Selection

The Phase II award selection was completed on schedule for the tenth consecutive year. A record 70 projects were chosen for awards out of 180 grant applications submitted. Twenty-four of these began their projects in February 1993, in our early submission procedure, with no gap in funding between Phases I and II. The Department of Energy continues to be the only agency that allows its awardees the opportunity to achieve funding continuity. The 70 Phase II awards are in 19 states and average about $500,000 for a two-year period. The technical topic areas with the most awards are Technology and Instrumentation for High Energy Accelerators (eight) and Advanced Industrial Sensors, Instrumentation, and Control Systems (seven).

SBIR Program Holds Meetings on Commercialization Assistance

Fifty-eight people from 50 companies with SBIR Phase II projects attended the Kick-Off Meeting on January 11, 1993 in the Germantown auditorium for the Department's third Commercialization Assistance Project. The primary purpose of the project is to accelerate the rate of commercialization of SBIR-funded technologies by providing individual assistance to Phase II awardees in the development of a business plan. The objectives of the meeting were to (1) explain in detail the effort that will be required of each SBIR awardee in the business plan development phase and (2) answer questions from the companies concerning the project. A training manual, entitled "Business Planning for Scientists and Engineers," was presented to each awardee at the meeting. This document was prepared by Dawnbreaker of Rochester, NY, the grantee for the project.

Companies that produce the best 23 business plans were invited to participate in the subsequent phases of the project. As part of this process, representatives from the 23 companies attended an Advanced Commercialization Workshop in Germantown, Maryland, on May 22-23, 1993. The primary purpose of the workshop was to accelerate the rate of commercialization of Small Business Innovation Research-funded technologies by providing individual assistance to Phase II awardees in the development of a business plan. At the workshop, each company improved its business plan, with individual help from the Dawnbreaker staff. In addition, the firms clarified their commercialization strategy and developed a sound rationale for payback to potential investors.

The culmination of the Department's third Commercialization Assistance Project was a Commercialization Opportunity Forum on September 28-29, 1993, at the Sheraton Premiere Hotel in Tysons Corner, Virginia. At the Forum, 24 companies that have received Phase II awards from the Department's Small Business Innovation Research program presented their business opportunities to 56 potential funding sources from either large corporations or venture capital firms. The 24 companies are attempting to either license their technology, form a joint venture, obtain venture capital, or develop some other form of strategic alliance.

SBIR Program Receives Compliments

An article on the reauthorization of the SBIR program appeared in the business section of the November 30, 1992, *Washington Post* and has been syndicated in newspapers across the country. The article contained an explanation of SBIR and was very complimentary to DOE's program. Two of the Department's best SBIR Phase III success stories were highlighted: Advanced Technology Materials, Inc. of Danbury, CT, for development of a filter to purify gases in the production of semiconductors and solar cells, and Manufacturing and Technology Conversion International, Inc., of Columbia, MD, for a process to convert coal into clean-burning gas.

SBIR Awardee Tops $3 Million in Non-Federal Revenues

Biolog, Inc., of Hayward, California, has achieved outstanding success in commercialization of its products, which were developed in a DOE SBIR project that began in 1988. Since May 1990, sales and equity investments from private investors have totaled more than $3 million. Almost 95% of this amount is derived from sales. The SBIR award to Biolog was for work of interest to the Office of Health and Environmental Research program on Deep Subsurface Microbiology. Biolog developed kits which help to characterize and identify bacteria that could be useful for the biodegradation of pollutants around weapons manufacturing sites. The Biolog test kit for bacteria identification is fast, easy to use, relatively inexpensive, and has the potential for identifying all bacteria. In 1991, Biolog received an "R&D 100 Award" as a result of research performed for the DOE SBIR project. Biolog has stated that the DOE SBIR award has contributed significantly to the development of commercial products from its technology and to its success in generating additional funding.

Three SBIR Projects Win R&D 100 Awards

Three companies with Small Business Innovation Research projects have received awards from *R&D Magazine* on its list of the 100 technologically most significant new products of 1993. Ten Small Business Innovation Research companies have now been honored with this award in the last six years. This year's winners are the following: (1) Chromex, Inc. from Albuquerque, NM for a vibrational molecular Raman spectroscopy technique, based on a 1991 award from the Office of Basic Energy Sciences/Division of Chemical Sciences, (2) North Star Research Corporation, also in Albuquerque, for a nested high voltage Tandem accelerator, based on a 1990 award from the Office of Health and Environmental Research, and (3) TeleRobotics International, Inc. from Knoxville, Tennessee, for an omnidirectional viewing and inspection system for fusion reactors, based on a 1992 award from the Office of Fusion Energy.

Integration With Energy and Technology Programs

Integrated Research Highlights

The Department of Energy has established strong programs in basic energy research, applied energy research, and technology development and deployment. By fostering the integration of these programs, the Department ensures that energy technology development is being conducted with benefit from state-of-the-art scientific knowledge and that the basic research programs are focused in areas directly relevant to Departmental missions. The Department possesses many effective forms of R&D integration, due in large part to the strengths of its national laboratories and the ability to collocate research and development activities at these sites. Provided below are some examples of research results where Basic Energy Sciences projects have been effectively integrated with other Departmental programs.

Ultrasensitive Detection Method Helps Support Nuclear Nonproliferation

Basic research in actinide spectroscopy and photophysics, supported by the Office of Basic Energy Sciences/Division of Chemical Sciences at the Argonne National Laboratory, has led to the development of an ultrasensitive signature method for detecting clandestine reprocessing of recently irradiated uranium targets for the production of nuclear weapons material. The development of this new method is funded by the DOE Office of Arms Control and Nonproliferation. In the new method, a pulsed near-ultraviolet laser is used for the unique excitation of trivalent curium ions in aqueous solution. Time and wavelength resolution of the resulting fluorescence emission from the curium excited electronic state ensures high specificity in this non-destructive analysis. This new method is a thousand-fold improvement in detection sensitivity in comparison with alpha radiation counting, the best current method. The isotope of interest is Cm-242, which has a 162 day halflife.

Biomimetic Program Featured in the *R&D Magazine*

The May 1993 issue of *R&D Magazine* contains a feature article on biomimetics, the synthesis of new materials using or mimicking nature's processes. An Office of Basic Energy Sciences/Materials Sciences Division program at the Pacific Northwest Laboratory is highlighted in the article as an example of the advances being made in this new area of science.

One aspect of the Pacific Northwest program involves the use of thin organic films to control the deposition and adhesion of ceramic thin films in a manner that mimics the principles of biological hard tissue formation (teeth, bone, and shells). Based on the ideas and principles developed in this research program, a Cooperative Research and Development Agreement was signed (Spring, 1992) with General Motors to make hard coatings for components of an automobile fuel delivery system. The Department of Energy's funding for this agreement was provided by the Office of Energy Efficiency and Renewable Energy, who recognized the potential of the Materials Sciences/Basic Energy Sciences program to produce inexpensive hard coatings on complex shapes while producing no hazardous wastes.

<u>Effective Integration of Basic and Applied Geosciences Research*</u>

Investigators at Brookhaven National Laboratory, Los Alamos National Laboratory, and the Mobil Exploration and Production Technology Center in Dallas are illustrating how basic and applied research in Department of Energy Laboratories can be integrated with, and coupled to, industry needs.

Dr. Mary Coles at Mobil is computing high resolution microtomograpic data on drill core samples for image reconstruction in conjunction with Dr. Per Spanne and Dr. Keith Jones at Brookhaven. Per, Keith, and Prof. Brent Lindquist (State University of New York-Stony Brook) are funded by the Office of Basic Energy Sciences/Geosciences Program to investigate potential use of synchrotron radiation for computed microtomography in the analysis of pore and fracture structure at the sub-10 micrometer level. For example, the second inset picture of this booklet* displays a typical pore space volume (light region) for a 200 micron region of Berea sandstone. In turn, the data are being used in two joint industry-lab partnerships involving Dr. Ken Eggert at Los Alamos National Laboratory and Dr. John Buckles and Dr. Coles at Mobil, funded by the Office of Oil and Gas (Office of Fossil Energy) and the High Performance Computing Program (Office of Scientific Computing) to use the data in transport models for improved oil recovery. Basic capabilities at the Brookhaven National Synchrotron Light Source are supported by the Office of Basic Energy Sciences/Chemical Sciences Division. The participation and leadership by a researcher at Mobil assures industrial understanding and "real-time" use of the results of basic research.

<u>Basic Studies at Ultra High Pressure Lead to Defense Programs Funding of Chemical Explosive Materials</u>

In the 1970's, the Office of Basic Energy Sciences/Division of Materials Sciences began a program at Los Alamos National Laboratory to study the behavior of materials under high-pressure and temperature. The goals of this research were to examine molecular materials of strategic importance to the Department of Energy national security and energy programs. The scientific approach was to develop and advance high-pressure technology in conjunction with theory to advance our understanding. Specifically, the aim was to study the physical and chemical transformations that occur at extreme pressures and temperatures.

The technology has advanced to the point that pressures can be determined in diamond-anvil cells at high temperatures with sufficient precision and over a wide enough range of pressures and temperatures to enable accurate measurements of the equations of state of fluid mixtures. Several spectroscopic pressure scales have also been developed, calibrated, and cross-correlated. The first practical theory to calculate chemical equilibrium in multi-component systems has also been developed.

Studies of fluid mixtures are important for knowledge of practical reasons in addition to the fundamental knowledge gained in this program. Knowledge of low-pressure phase equilibria of fluid mixtures is important for this development of new separation techniques for the petrochemical industry. Similarly, supercritical fluids can be used as solvents for a variety of chemical processes such as the use of supercritical water to destroy chemical wastes. At somewhat higher pressures, geochemists rely on high-pressure, high-temperature experiments to understand problems in fluid migration in the earth. At higher pressures yet, a knowledge of the equations of state of fluid mixtures is absolutely essential for understanding and predicting the behavior of chemical explosives.

The science and technology developed with the Division of Materials Sciences funding is now being applied to determine the equation of state of fluids composed of real detonation reaction products. This problem is of central importance to the Department of Energy Defense Programs and funding from this part of the Department of Energy will carry the work forward as the Division of Materials Sciences funding phases out.

Chemical and Engineering News Article Highlights Hanford Tank Farm Safety

An article appearing recently in *Chemical and Engineering News*, a weekly publication of the American Chemical Society, on issues involving the Hanford tank farm castigated DOE and Westinghouse for numerous deficiencies in their handling of the waste farm at Hanford. However, one bright spot was found: "DOE and Westinghouse get higher marks for progress in understanding what is happening inside the tanks to generate explosive gases, especially the large release of hydrogen gas from tank 101-SY and smaller releases in 22 other tanks. The team reports that 'progress is being made in duplicating and understanding the compounds formed in the radiolytic decomposition of organics in the tank.'"

Thomas Dunning from the Molecular Sciences Research Laboratory at Pacific Northwest Laboratory and Philip Horowitz of the Chemistry Division at Argonne National Laboratory, both supported by the Chemical Sciences Division/Office of Basic Energy Sciences, co-chaired the Tank Waste Science Board, the group that was responsible for the research work cited in the *Chemical and Engineering News* article. In addition, the Radiation Chemistry group under the leadership of Dr. Daniel Meisel at Argonne was instrumental in unraveling the gas formation mechanism. The success of this team's effort in a very short time highlights the importance and value of the Department's ongoing basic research efforts, not only for the knowledge that is generated by the research itself, but for the resident expertise that can brought to bear rapidly and effectively on the major problems of the Department of Energy.

Neutron Dosimetry Data from the HFIR Pressure Vessel Yields Insight to Embrittlement Issue

The Nuclear Regulatory Commission and the Materials Sciences program jointly sponsored the first comprehensive neutron dosimetry experiment on the region of the High Flux Isotope Reactor (HFIR) pressure vessel from which much of the earlier embrittlement data was obtained. Prior to this new dosimetry experiment, the only measurements of neutron fluxes at the pressure vessel were those obtained from activation of nickel and iron in stainless steel monitor wires from surveillance packages, which yielded the fast flux >1 MeV; thermal fluxes were estimated. The new dosimetry experiment included thermal flux monitors as well as three different monitors for fast flux. Measurements of fast flux from nickel wires agreed with the measurements from the stainless steel monitors in the surveillance packages. Surprisingly, the fast flux measured by beryllium and neptunium monitors in the experiment was 15 times larger than that measured by the nickel monitors, suggesting that the spectrum may contain a hitherto unsuspected population of neutrons in the range 0.5 to 2 MeV, just below the threshold energies for recording by nickel and iron monitors. Measurements from five different thermal flux monitors all agreed with one another and verified recent calculations. (Note that original estimates suggested a strongly thermalized spectrum and made the neutron spectrum a major suspect in causing the embrittlement. However, more recent calculations indicated that the spectrum was not as strongly thermalized).

This experiment confirms that the neutron spectrum at the site of accelerated embrittlement measurements is not strongly thermalized and, hence, implies that thermal neutrons are not a major factor in the accelerated embrittlement. The measurements also raise the tentative possibility that the stainless steel monitors in the surveillance capsules are underestimating the fast flux, and therefore, the embrittlement is not really accelerated but is simply misrepresented by the earlier reliance on fast fluences from the stainless steel wires. Additional dosimetry measurements are now underway to explore this possibility. These results are also pertinent to concerns about the integrity of commercial power reactor vessel support structures.

This research was performed by K. Farrell, S. T. Mahmood, R. E. Stoller, L. K. Mansur, F. B. Kam, C. A. Baldwin, F. W. Stallman, L. Robinson, F. F. Dyer, and F. M. Haggag, ORNL, and B. M. Oliver, Rockwell International Corp. It was jointly supported by the Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission and the Division of Materials Sciences, Basic Energy Sciences, Department of Energy.

Basic Chemistry Research on Separations Results in Facile Analysis for Actinide Elements

A known analytical method for the separation of actinides from high level waste mixtures has now been developed into a fast and highly accurate technique for the analysis of actinide contaminants in biological and environmental samples. The analysis is based on the versatile extractant, octyl (phenyl)-N,N-diisobutylmethylphosphine oxide, (CMPO) which was synthesized by a BES/Chemical Sciences-funded group in the Chemistry Division of the Argonne National Laboratory and is the basis for the TRUEX process. In both the separation and the analytical method, the extractant is incorporated into a macroporous resin to produce a solid, stationary phase through which the acid solution containing the actinides is passed. The actinides are first deposited on the resin bed. The analytical technique is based on selective and sequential elution of each actinide element by designed solvent systems through the small-sized elution columns and analyzed by routine counting techniques. The procedure requires but a single extraction column of 10-20 milliliters capacity for five important actinides. The small same volume greatly simplifies the process and reduces the cost of the analyses of actinides in laboratories, especially where there is a high sample load as with biological and soil samples. The loaded and ready-to-use columns are currently marketed by Eichrome Industries, a spin-off company from the BES basic research project. This analytical technique is now in the implementation stage with funding from DOE's Office of Environmental Restoration and Waste Management (EM).

Ames Laboratory Develops New Waste Cleanup Characterization Technology

A mobile analytical laboratory was displayed by the Ames Laboratory at the Environmental Protection Agency Region 7 Superfund Site Managers meeting on December 9, 1992. The instrumentation for this mobile laboratory was based on the inductively coupled plasma-atomic emission spectroscopy (ICP-AES) basic research supported by the BES/Chemical Sciences Division more than a decade ago, and was developed by the Office of Environmental Restoration and Waste Management (EM). The ICP-AES analytical technique was described in DOE This Month, January 1987. A recent demonstration of this mobile laboratory at Fernald, Ohio in September produced very promising results. The on-site capabilities of this laboratory of rapid and remote monitoring of heavy metal contaminants were demonstrated. Mapping of contamination is the first important step to timely and cost-effective environmental remediation of DOE and EPA superfund sites. The Iowa Department of Natural Resources has shown considerable interest in this new technology which can speed the cleanup of EPA superfund sites around the state.

Fundamental Geochemistry of Geothermal Brines Aids Fluid-Rock Models

Aluminum is the third most abundant element in the Earth's crust and aluminosilicates play a major role in determining the chemistry of brines in sedimentary basins and geothermal systems. Heretofore, the geochemistry of aluminum has been poorly characterized due to (i) exceedingly low solubilities, (ii) extremely sluggish dissolution and precipitation rates, and (iii) tendency of Al to form complex species. The thermodynamic properties of Al^{3+} and $Al(OH)_4^-$ and the solubility of gibbsite have been determined over the range 0°-100°C and 0.1-5.0 molal NaCl. The experiments were conducted over a period of two years with each equilibration taking several weeks to several months. This study represents the most extensive series of measurements of Al speciation in high temperature brines in existence at this time. The results have been incorporated into major computer codes designed to model fluid-rock interactions over a broad range of geochemical conditions. This information is critical in modelling the effects of dissolution and precipitation during diagenesis and alteration, petroleum migration, geothermal fluid flow, and nuclear waste storage.

This project was supported by the Geosciences program of Basic Energy Sciences and in part by the Geothermal Technology Division of Conservation and Renewable Energy because of its specific applications to geothermal industry.

Fracture Properties of Superconducting Sensor Improved by Argonne-Illinois Superconductor Collaboration

A simple and inexpensive glazing technique was developed which improves the fracture toughness of oxide superconductor liquid level sensors. Due to the intrinsically low fracture toughness of oxide superconductors, both packaged and unpackaged cores are very brittle and cannot survive bending stresses caused, for example, by handling or thermal stresses. The glazing technique developed by the Argonne-Illinois Superconductor group does not affect the superconductivity and can increase the load to fracture by a factor of four. In addition to providing a surface compressive stress, the glass seals the superconductor which prevents environmental degradation. Since the glass has a low thermal conductivity, the glass also reduces the heat conduction through the dipstick, thereby reducing the rate of loss of the cryogen. This work was performed by Drs. W. Wu, C.-Y. Chu, K. C. Goretta and J. L. Routbort of Argonne National Laboratory with support from Conservation and Renewable Energy and from BES-Materials Sciences and in collaboration with Mr. J. D. Hodge and Mr. D. S. Applegate of Illinois Superconductor Corporation.

In Situ Vitrification Tested as Potential Method for Remediation of Contaminated Soils

In situ vitrification (ISV) transforms permeable, easily leached, contaminated soils into low permeability, leach-resistant vitreous and crystalline materials via in situ resistance heating. A comprehensive test of ISV was conducted at the Oak Ridge National Laboratory in May 1991 as an integrated project funded by Environmental Restoration and Waste Management and Basic Energy Sciences. The principal investigators were G. K. Jacobs, N. W. Dunbar, M. T. Naney (Oak Ridge National Laboratory), R. T. Williams (University of Tennessee). This test provided important new constraints on the ISV process and its application to stabilizing contaminated soil under actual field conditions. The results of this research define the growth and cooling structure of the melt using geophysical data and quantify the volatiles and particulates emitted from the growing melt with geochemical analyses. This ISV experiment also provided an analogue to natural magmatic systems on a scale not usually available to scientists. These results place important engineering constraints on the application of ISV to contamination remediation and geological constraints on the application of ISV to contamination remediation and geological constraints on the process of magma generation and differentiation. The results were reported in the lead article of EOS, the weekly newspaper of geophysics on September 22, 1992. They serve to emphasize the benefits of jointly planned projects involving ER and other DOE offices. ISV is produced by applying electrical power to the ground through four graphite electrodes. A hood is placed over the melt to collect gases and particulates released by the process. Melt formation was accompanied by vigorous bubbling and rapid convection in the melt. Bubble-forming gases were produced by a combination of devolatilization processes (H_2O and CO_2) and reduction at the electrodes (CO and CH_4). Halogens, alkali elements and trace metals were sublimated in ratios similar to that observed in volcanic systems. Early stage vertical growth of the melt mass with late stage horizontal growth is consistent with the greater horizontal convective heat transfer as the melt grows. The bulk of the ISV rock underwent a 50 percent reduction in volume and was almost completely crystalline with glass present only in the upper portions where cooling was most rapid. Seismic data show an altered soil zone around the ISV mass and the presence of major heterogeneities within 12-15 hours after termination of power coinciding with crystallization fronts.

World Record Achieved for High Efficiency Solar Cell

An exciting new world record efficiency of 29.5 percent has been obtained for a solar cell comprised of a gallium-indium phosphate/gallium arsenide monolithic tandem. The work was done in the National Renewable Energy Laboratory's III-V group headed by Jerry Olson. This is the highest one-sun efficiency measured to date for any photovoltaic device, and is a substantial improvement over the previous highest efficiency of 27.6 percent.

This cell has several advantages for concentrator applications. The main one is that the current density is roughly half that of a comparable gallium arsenide concentrator cell. Consequently, the energy losses for this tandem cell are reduced by a factor of four. This relaxes the design constraints for the collection grid conductivity, the emitter sheet resistance, and the tunnel diode conductivity. One of the factors which plays a key role in device optimization is control of the band gap of the top cell material, gallium-indium phosphate. The band gap of this material is a sensitive function of the ordering parameter. The basic research on the ordering phenomena in gallium-indium phosphate is supported by the Office of Basic Energy Sciences/Materials Sciences Division, the technology of solar cell development is supported by the Photovoltaics Division at Energy Efficiency and Renewable Energy, and the transfer of this technology to the private sector is being accomplished through collaborative development work supported by industry.

Planning and Information Transfer

The Department is focusing on improving integration of programs to become a more effective organization. Ensuring that support for science and technology are better coupled will provide a better return on the taxpayer's dollars. The most effective mechanisms for integration are strong coordination and planning activities between programs at headquarters, collocation of researchers, open communication from all stakeholders, and in-depth workshops and conferences between scientists, engineers, and technologists with management sponsorship and participation. Many of these mechanisms are already in place, and some examples of such planning and information transfer activities involving Basic Energy Sciences are presented below.

Energy Materials Coordinating Committee Annual Report

The Energy Materials Coordinating Committee Annual Report for 1993 has been issued. The Energy Materials Coordinating Committee provides a means for enhancing information transfer and coordination between the Department of Energy's various materials programs. In its 1993 Report, the Energy Materials Coordinating Committee made a major effort to improve the accessibility and usefulness of the report to persons seeking information by the Department of Energy's materials-related programs. Redundant program and project descriptions were eliminated, and project descriptions were shortened. By sharing of budgetary and program information and by fostering contacts between program managers, the Energy Materials Coordinating Committee seeks to further the effective use of materials expertise within the department.

The report presents a budgetary summary of the Department of Energy material activities for FY 1992. Funding for these activities by Assistant Secretarial Office are:

Office of Energy Efficiency and Renewable Energy	$ 99,060,000
Office of Energy Research	298,503,852
Office of Environmental Restoration and Waste Management	20,015,000
Office of Nuclear Energy	156,262,000
Office of Civilian Radioactive Waste Management	700,000
Office of Defense Programs	78,597,000
Office of Fossil Energy	6,614,000
TOTAL	$659,751,852

The Energy Materials Coordinating Committee promotes the transfer of information and coordination through seminars sponsored by its six subcommittees and by publishing its annual report. The Energy Materials Coordinating Committee annual report is provided as a service to the Department of Energy, to other Federal Agencies and to interested members of the public. Copies of the 1993 report may be obtained by calling Christie Ashton, (301) 903-3427.

Meeting to Develop a New Approach for Environmental Research and Development

Dr. Steven G. Barnhart of the Office of Basic Energy Sciences/Chemical Sciences Division, attended a meeting of the Working Group to Develop a New Approach for Environmental Research and Development at the Department of Energy on Friday, September 17, 1993. The purpose of this meeting was to "bring together individuals from the National Laboratories, Operations Offices, DOE Headquarters organizations, and other agencies to provide input in developing a process for managing and coordinating environmental technology development across DOE."

Large-Scale Computer Simulations Discussed at Research Assistance Task Force Meeting

A Research Assistance Task Force entitled "Evaluation of Interatomic Potentials for Large-Scale Simulations of Non-Equilibrium Phenomena in Silicon Carbide," was co-organized and supported by the Offices of Basic Energy Sciences ($25,000) and Fusion Energy ($10,000). The workshop took place in Santa Barbara, California, on August 22-25, 1993, and was co-chaired by Dr. M. W. Guinan of Lawrence Livermore National Laboratory and Professor Nasr M. Ghoniem of the University of California at Los Angeles. Of the fifteen invited participants, six were from universities, four from National Laboratories, two from private sector industry, and three from outside the United States.

The purpose of this Task Force was to determine what additional features need to be added to existing semi-empirical potentials, what experimental and first principal calculational results should be used as input, and whether the resulting potentials will allow large scale simulations on near term computer architectures. The development of tractable and accurate semi-empirical potentials for strongly covalent materials would allow the start of large scale molecular dynamics calculations for the study of radiations effects, fracture, nanophase properties, and surface microstructure of these important materials.

Calculations using existing semi-empirical potentials revealed that different potentials give very different results for defect configurations and energetics and for displacement damage processes. It was generally agreed that there is an urgent need for more experimental data and/or ab-initio theoretical results for a well-defined set of defect properties in silicon carbide. This information is required to validate semi-empirical potentials before proceeding to initiate large scale simulations. The participants agreed to carry out an informal comparison of simple defect properties predicted by four different forms of semi-empirical potentials with those obtained from advanced tight-binding models. The summary report of this evaluation will be published in the journal, *Modelling and Simulation in Materials Science and Engineering*.

Innovation in Materials Processing and Manufacture: Exploratory Concepts for Energy Applications

A Workshop on Innovation in Materials Processing and Manufacture: Exploratory Concepts for Energy Applications was held on March 11-12, 1993, at Oak Ridge National Laboratory. The workshop was sponsored by the Office of Basic Energy Sciences/Division of Advanced Energy Projects. The goal was to identify potential research areas for the Division's program that are in need of novel concepts, with a focus on materials and manufacturing. The workshop attracted considerable interest from industry, academia and national laboratories. The final list of invitees reached about 70. Participants represented several Department of Energy offices as well as the Office of Science and Technology Policy, the Environmental Protection Agency and other agencies. Seven Working Groups on quite diverse energy-related topics identified research areas, many of which can be approached from several disciplines.

They include: surfaces, interfaces, coatings, bonding, joining (including the need for new tools for characterization and study); novel approaches to parts fabrication (such as integrated methods, process efficiencies); opportunities for revolutionary materials performance (ranging from biopolymers and catalytic antibodies to nanophase composites, smart materials, and self-reinforcing materials); lubricants (including petrochemical replacement and environmental- and recycling problems); fabrication of new electric devices using nonconventional approaches (such as thermoelectrics for heating and refrigeration and functional proteins that yield electron transport or electronic switching); and alternative energy approaches (removal of mercury from coal; hydrogen gas production; and "clean" alternatives for cars).

General Purpose Computer Program Developed for Structural Analysis

Convenient, quantitative methods for the structural analyses of thin films and superlattices, two important configurations now being used in a number of applications, including electronic devices, magnets, and superconductor devices, have generally been unavailable. Such a method has now been developed by Professor Ivan Schuller of the University of California, San Diego, and made available in the form of a general purpose computer program to other investigators in the field. The program is provided free-of-charge with the proviso that the user reference the publications describing the development of the model and acknowledge that the refinement program was developed with funds provided by the Department of Energy. To date, the program has been supplied to approximately 100 scientists world-wide.

Working Group Discusses Research on Ceramic Composites

Dr. Alan Dragoo, of the Division of Materials Sciences, participated in the recent Working Group Meeting on Continuous Fiber Ceramic Composites (CFCC) held by Energy Efficiency, EE-221, in Chicago on November 18-19, 1992. Industrial, Federal laboratory, and university participants in the CFCC program reported on the initial activities, accomplishments and project plans for their various research efforts. The program is divided into an industrial component (Task I) and a Federal laboratory/university component (Task II). Work under Task I addresses the processing of ceramic components for particular end-use applications such as high-temperature gas turbines and filters. The effort under Task II addresses materials characterization and basic science issues. CFCC's, like most composites, are by the nature of their construction and composition inherently nonequilibrium systems and, hence, potentially dynamic systems which can be expected to change in time with respect to elemental and phase distribution and strength and toughness. An engineering objective is to minimize deleterious changes. A further engineering objective is to measure design parameters such as modulus of rupture and flexural strength for determination of product quality and prediction of component lifetime. A scientific objective is to understand the mechanisms by which changes occur and to model those changes accurately as a function of temperature, load and environment. The remarks of several research groups in the CFCC program indicated that models for lifetime prediction are critically needed to guide material design and for the meaningful use of design data.

Meeting of the Emerging Energy Technology Coordination Group

The meeting of the Emerging Energy Technology Coordination Group was held on September 13, 1993, in Room G-426, Germantown. The group meets approximately every quarter and presently includes representation from the Office of Energy Efficiency and Renewable Energy's Office of Industrial Technologies; Office of Basic Energy Sciences/ Division of Advanced Energy Projects; and the Office of Fossil Energy's Office of Advanced Research. Participation by interested parties is welcome. The agenda for this meeting included a presentation on planning methodologies of the Office of Industrial Technologies and an overview of the Defense Program's Technology Transfer program. This was followed by a report on an Advanced Manufacturing Program meeting of August 27, 1993, held in Detroit; a survey of interests among the represented offices in thermophotovoltaics; and a discussion on mechanisms or processes to achieve coordination for specific topical examples.

Environmentally Conscious Synthesis, Processing, and Use of Ceramics

A Research Assistance Task Force entitled "Environmentally Conscious Synthesis, Processing, and Use of Ceramics" was jointly sponsored by the Advanced Industrial Concepts/Office of Industrial Technology of Energy Efficiency and Renewable Resources and the Division of Materials Sciences/Office of Basic Energy Sciences and took place on May 5-7, 1993, at Princeton University. The 34 invited participants included 21 from universities, 9 from industry, and 4 from the Department of Energy laboratories. A detailed summary including recommendations for research directions is published in the *Journal of the American Ceramic Society*.

Discussions focused on environmental issues ranging from binder and solvent removal to water-based processing and minimization of airborne particulates; novel processing techniques including biological mimicking; the use of ceramics for minimization of waste effluent and the identification of key issues that must be understood in order to bring about environmentally conscious technology for industrial ceramic processing.

A major finding was the potential to solve many environmental problems through the use of submicron powders without binders, surfactants, or solvents. This technology, however, requires a basic understanding of particle-particle interactions during processing, which currently does not exist. The ability to control or tailor these interactions was identified as critical for the United States ceramic industry to achieve environmentally conscious processing. The deliberations also included recommendations regarding net-shape forming for the minimization of the production of airborne particulate, and the use of ceramics in ion-exchange chemical separations, catalysts and supports, high-temperature fuel cells, and emission control.

Environmental Workshop Held at Stanford Synchrotron Radiation Laboratory

A very useful workshop focusing on synchrotron radiation-based techniques applicable to environmental issues was held at the Stanford Synchrotron Radiation Laboratory, which is supported by the Office of Basic Energy Sciences, on May 24-25, 1993. The workshop concentrated on the use of X-ray Absorption Spectroscopy for chemical speciation of dilute levels of toxic and radioactive elements in complex solids such as contaminated natural soils. In addition to lectures, the workshop featured both "hands on" data collection using Stanford Synchrotron Radiation Laboratory beam lines and data analysis sessions. It drew 37 people from 21 institutions, including a number of National Laboratories. Several participants brought samples pertinent to their own research, for which X-ray Absorption Spectroscopy data were collected and analyzed during the course of the two days. Most of the attendees were novices in the use of synchrotron radiation to study these problems and their enthusiasm for using these techniques was apparent.

Workshop Examines the Changing DOE Engineering Mission and Priorities

On August 18, 1993, Dr. O. Manley, Engineering Research Program, Office of Basic Energy Sciences, attended a one-day workshop at Dallas, Texas, dealing with the potential role that DOE labs and production facilities can play in the emerging DOE Engineering Initiative. The Secretary is to be briefed on this endeavor by Energy Efficiency early next month. The meeting was attended by about twenty representatives from various weapons, multipurpose and single purpose DOE laboratories. The all-day meeting centered on how the laboratories could be organized to maximize their usefulness to U.S. industry under the expected effort. The discussions focused on the need for forming programs in core competency areas with sustained long-term support from which, as needed, application teams could be formed to address specific industrial problems which fall within DOE's mission. Some effort was expended on how such a program should be managed at DOE headquarters. It was suggested that it might be confined to a single office, preferable at the Assistant Secretary level with its own budget. The functions of such an office would be coordinated across the Department.

Review of Energy Superconductivity Technology Program

Bob Gottschall of the Office of Basic Energy Sciences/Materials Sciences Division served as one of the external reviewers of the above superconductivity program on July 28-29, 1993. It consisted of research at five DOE laboratories, three private sector industrial organizations and one university sub-contractor. Bob is pleased to report that there is excellent interfacing and coordination between the Basic Energy Sciences and the Electric Energy Systems superconductivity activities at the five laboratories where both programs are co-sited.

Mini-Symposium Highlights the Laboratory High-Rate Metal Forming Technology

High-rate metal forming is an enabling technology that will permit low cost fabrication of automotive body components with a minimization of waste material and costly machining, which is of critical importance to the success of the United State Automotive Materials Partnership and the United States Council for Automotive Research initiative. It also is a technology that has been developed, advanced and utilized at five Department of Energy National Laboratories, with each having unique personnel, instrumentation or computer modeling capabilities. These laboratories are: Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory, Pacific Northwest Laboratory, and Sandia National Laboratories. Representatives from each of these national laboratories made a presentation of their capabilities and past achievements in this subject on July 14, 1993, in a half day Mini-Symposium that was sponsored by the Office of Basic Energy Science's Center of Excellence for the Synthesis and Processing of Advanced Materials. The participants included Department of Energy personnel from the offices of Energy Efficiency and Renewable Resources, Science and Technology, Basic Energy Sciences, and the participating national laboratories. A meeting on the subject will be planned with industry in the Fall of 1993.

Advanced Neutron Source (ANS) Public Scoping Meeting for the Environmental Impact Statement (EIS)

The third and last public scoping meeting for the ANS EIS will be held at Los Alamos, New Mexico, June 30. The other two, the first at Oak Ridge, Tennessee, and the second at Idaho Falls, Idaho, were very supportive. No major issues were brought up by the citizens. The Oak Ridge meeting had about 160 participants and the Idaho Falls meeting had much fewer participants. Energy Research is working with Nuclear Energy on these meetings.

Conference Highlights Need to Better Understand the Formation of Nitrogen Oxides

The Fifteenth annual Department of Energy Combustion Research Conference, sponsored by the Chemical Sciences Division of the Office of Basic Energy Sciences and hosted by Brookhaven National Laboratory, was held from June 2-4, 1993, at Lake Harmony, Pennsylvania.

As in the past, the opening presentation was by someone unconnected with the Department of Energy but with strong interests in Department efforts in this area. This year's speaker was Dr. Daniel J. Seery, Manager of Combustion Science at the United Technologies Research Center. Dr. Seery's presentation strongly emphasized the need for fundamental studies of the formation of the oxides of nitrogen in gas fired turbines which are becoming the system of choice for electrical power generation. In spite of decades of study, the mechanism for formation of the oxides of nitrogen is still poorly understood and so strategies for their removal are difficult to formulate. Dr. Seery's talk provided an excellent framework against which the technical presentations could be reviewed.

In addition to nearly 100 contractors and grantees, the meeting was attended by representatives from the Office of Fossil Energy, combustion related industries, and other Federal programs. Representatives from the Office of Energy Efficiency and Renewable Energy were invited to participate, but were unable to attend. The purpose of these annual meetings is to encourage collaboration, cooperation, and exchange of current research ideas among those grantees and contractors supported by the Office of Basic Energy Sciences whose research is related to the general area of combustion.

Heavy Duty Transportation Technologies Discussed at Combustion Coordinating Group Meeting

The Combustion Coordinating Group consisting of representatives from the Department of Energy Offices of Energy Research, Defense Programs, Energy Efficiency and Renewable Energy, and Fossil Energy met on June 8 to hear a presentation on the Heavy Duty Transportation Technologies program of the Office of Energy Efficiency and Renewable Energy. The program covers a broad range of incremental changes in diesel engines designed to meet challenging emission and energy efficiency goals by the year 2000. Examples of interprogram technology transfer were examined, particularly in the development of combustion models and fuel additive techniques for control of oxides of nitrogen emissions. In a separate discussion, the representatives from the Office of Fossil Energy and the Office of Energy Research have agreed to explore a joint effort in the development and application of combustion models. The Combustion Coordinating Group meets once a month to explore opportunities for enhanced integration of the Department's programs in combustion-related research and in the development of advanced combustion systems. The Office of Energy Research representative is William Kirchhoff of the Office of Basic Energy Sciences, Chemical Sciences Division.

Division of Materials Sciences Participated at the Conference on Fossil Energy Materials

Materials Sciences was represented at the Fossil Energy Materials Contractors Review at Oak Ridge on May 11-13, 1993, by Dr. John N. Mundy. Six of the contractor participants are also funded by Basic Energy Sciences with a total of $2.6 million. The Fossil Materials Program addresses materials requirements for all fossil energy systems, including materials for coal processing, coal liquefaction, coal gasification, heat engines and heat recovery, combustion systems, and fuel cells. The 16 ceramics papers presented at the conference concerned synthesis, coatings, and composites, with added concerns of joining, interface interactions and high temperature mechanical properties. The 21 papers on new alloys concerned alloy development, fabrication, welding, processing, environmental effects and of course high temperature mechanical behavior.

Combustion Research Coordinating Group Formed with Department-Wide Participation

Recognizing the need for more frequent communication between offices in the Department in the area of combustion research, representatives from the Department of Energy Offices of Energy Efficiency and Renewable Energy, Energy Research, Fossil Energy, and Defense Programs have formed a Department wide Combustion Coordinating Group. The first meeting of the group was held on April 6, 1993, and the second meeting was held on May 11, 1993. All programs with plans and ongoing efforts in combustion research from basic to applied are welcome to join the group. Meetings are anticipated to be held on a regular, bimonthly basis or more frequently if required. Typical agendas will consist of presentations on present program activities and plans and general discussions on ways to improve the coordination between complementary efforts. Chairmanship of the group will rotate on an annual basis among the participating offices with William Kirchhoff, Office of Basic Energy Sciences/Division of Materials Sciences, serving as the current chair.

The agenda for the meeting of the Combustion Coordinating Group on September 20 consisted of only one item: a presentation by Dr. Julian Tishkoff and Dr. Mitat Birkan on the combustion-related programs at the Air Force Office of Scientific Research. The Department of Energy's representatives came from Fossil Energy, Energy Efficiency and Renewable Energy, and Energy Research. Within Energy Research, Basic Energy Sciences was represented by Dr. William Kirchhoff of the Division of Chemical Sciences.

Although many of the Air Force programs in combustion are unique to Air Force problems such as the interaction of chemistry and turbulence under supersonic conditions, there remained many areas such as fundamental chemistry and fluid dynamics that are common to both the Air Force and the Department of Energy. The discussion was lively and included expressed desire on the parts of both the Air Force and the Department of Energy's representatives to continue such meetings and to develop a forum for more broadly coordinating combustion research throughout the appropriate agencies and departments of the Federal Government. Viewgraphs and reports from that meeting will be circulated among the members of the Combustion Coordinating Group.

Proceedings Published for Research Assistance Task Force on Research Opportunities in Photovoltaic Semiconductors

The Photovoltaics Branch of the Office of Conservation and Renewable Energy and the Office of Basic Energy Sciences/Division of Materials Sciences jointly sponsored a Research Assistance Task Force on "Photovoltaic Materials: Innovations and Fundamental Research Opportunities," which was held July 27-29, 1992, in Vail, Colorado. The Task Force was organized and chaired by Dr. Alex Zunger of the National Renewable Energy Laboratory, Golden, Colorado. Seventeen scientists, well-known for their research in photovoltaic materials and semiconductors, participated in the Task Force (8 from universities, 4 from DOE laboratories, 4 from private sector industry, and 1 from abroad). The proceedings of this Task Force have recently been published as a special issue of the Journal of Electronic Materials (Volume 22, No. 1, January 1993). Opportunities and subtopics that are included in the proceedings are: New Materials and Structures of Photovoltaics, Polycrystalline Compound Photovoltaics, Linear Optical Response of Semiconductors, Hydrogenated Amorphous Semiconductors, Growth of Photovoltaic Semiconductors, Crystalline III-V Photovoltaics, and Silicon Photovoltaics and Defect Control. Besides providing a readily available source on the current understanding of photovoltaic materials, the proceedings contains insightful recommendations concerning the types of fundamental and applied research that could possibly lead to the technological development of devices for a more efficient photovoltaic exploitation of solar energy.

Integration with Environmental Restoration and Waste Management on Radioactive Waste Management

Two Office of Basic Energy Sciences/Chemical Sciences Program Managers, Drs. F. Dee. Stevenson and John L. Burnett, participated in a recent Waste Separations and Pretreatment Technical Review co-sponsored by the Office of Waste Management and the Office of Technology Development. Environmental Restoration and Waste Management programs under review were the Underground Storage Tank - Integrated Demonstration and the Efficient Separations and Processing - Integrated Program. To ensure better coordination of research and development programs between Energy Research and Environmental Restoration and Waste Management in these areas, Dr. Stevenson will serve on the Core Planning Group to assist in the design and research program content and Dr. Burnett will serve on the Technical Review Group to assist in the review and choice of research proposals submitted by investigators. Other members of both groups include scientists and engineers from other Department of Energy and university programs. Two meetings per year are tentatively planned for each group.

Energy Efficiency (EE)-Sponsored Alternative Feedstocks Workshop

Dr. C. R. Yonker of the BES/Division of Chemical Sciences represented BES at the EE-sponsored Workshop on Alternative Feedstocks which was held at Argonne National Laboratory on December 9-10, 1992. Representatives from 17 different industries, DOE, 4 DOE National Laboratories, and the U.S. Department of Agriculture attended and were asked for their input into formulating the areas of future development and emphasis in the alternative feedstocks program. It was acknowledged during the executive session that the BES research programs in basic separations science and metabolic pathways in microbe and enzymatic reactions are important to EE's goals for this program.

Presentations were made in the areas of bioprocess analysis and engineering, advanced processing concepts, and metabolic pathways in alternative feedstock production. Conclusions from this workshop include recommendations regarding future research aimed at understanding the production of the organic acids (lactic acid) and the need for long-term research to reduce the financial risks of industries in this area. Currently, the workshop proceedings are being cumulated for dissemination to the attendees and EE is formulating a working document defining its role in the alternative feedstocks area.

This was the third meeting between BES and EE in the areas of alternative feedstocks. An informational meeting was held on November 13, 1992, in which BES staff presented a description of basic research projects which are supportive of the EE program in alternative feedstock production. Further coordination between BES and EE will occur in future meetings and at a symposia which is currently arranged for Kansas City in May 1993.

Basic Studies in Radiation Effects Acknowledged by Fusion Materials Program

At the Fusion Materials Program review held at DOE/Germantown, November 24, 1992, speakers from four national laboratories acknowledged contributions of BES programs in fundamental studies of radiation effects to their efforts in materials development for fusion applications. Dr. Art Rowcliffe (Oak Ridge National Laboratory) cited basic studies and modeling of mechanisms in austenitic and ferritic steels, Dr. Russ Jones (Pacific Northwest Laboratory) referred to crack growth studies and modeling of SiC composites, Dr. Dale Smith (Argonne National Laboratory) noted baseline irradiation response studies of Nb and V alloys, and Dr. Gene Farnum (Los Alamos National Laboratory) acknowledged BES support for neutron damage studies in ceramics. BES was represented at the program review by Dr. Michael Guinan a detailee for the BES/Division of Materials Sciences.

Environmental and Molecular Sciences Laboratory (EMSL) will Better Integrate Energy Research (ER) with Environmental Restoration and Waste Management (EM)

A major construction review of the EMSL at the Pacific Northwest Laboratory (PNL) was held November 16-18, 1992, with a joint team of invited ER and EM reviewers. This review covered detailed discussions of the program areas to be addressed by the EMSL as well as an indepth look at the major scientific research equipment being developed and purchased for this facility. The consensus of the review team was that the EMSL will provide a critical basic and applied research capability directed toward the cleanup of the Hanford site. The review team encouraged the DOE to expedite the construction of the facility by anticipating and reconciling any barriers that may impede the progress toward bringing this world class facility to completion and operation.

Key Decision 2 (KD-2) for the EMSL at PNL was approved by Under Secretary of Energy Hugo Pomrehn on October 30, 1993. This decision provides authorization to begin detailed design of the EMSL and to initiate procurement of long lead equipment items. The Joint EM/ER Working Group met in November 1993 at PNL together with four teams of peer reviewers to critique the program research, and computer equipment plans for the EMSL. This is an EM construction project which will provide important new capability for ER research. The ER support for the facility is being managed by the Office of Health and Environmental Research.

Disposition of High Flux Isotope Reactor (HFIR) Spent Fuel

The Office of Facilities, Fuel Cycle and Test Programs, NE-47, as the managing office for the ER nuclear facilities, requested a Program Plan for the disposition of the accumulating spent fuel from HFIR. This Plan was submitted on September 1, 1992, and addresses several options for the shipping and storage of spent fuel elements that must be explored and implemented in a timely manner to avoid shutdown of the reactor. The options include leasing or construction of a shipping cask, expanded storage in the HFIR pool, and a new dry storage facility on the HFIR site.

Representatives from the Oak Ridge Field Office (OR), NE-47, and ER/BES met with the Office of Waste Operations (EM-351) to coordinate the Oak Ridge National Laboratory (ORNL) Program Plan for the disposition of the accumulating spent fuel from the HFIR with the DOE-wide EM Implementation Plan for Management of Spent Nuclear Fuel and Associated Facilities. Additional pool storage space, followed by on-site dry storage, must be made available at ORNL for HFIR spent fuel by February 1995 to avoid shutdown. This additional storage space will be needed before the EM plan is expected to be in place and the EM facility able to receive spent fuel. This coordination between ER, NE, EM, and OR is essential to ensure that the ER action for additional storage at ORNL is compatible with the overall EM Implementation Plan and to avoid as much as possible any duplication of effort. ORNL is proceeding with its Program Plan for Disposition of HFIR Spent Fuel and preliminary discussions with EM-351 suggest that the EM plan will be compatible with the ORNL Plan.

Further Interactions Between Basic and Applied Materials Research Programs

David Beecy and Jim Carr (Fossil Energy) met with Bob Gottschall and John Mundy (Basic Energy Sciences/Division of Materials Sciences) to discuss the applied materials programs supported by Fossil Energy to improve materials used in the processing, liquefaction, and gasification of coal, in heat engines and heat recovery, and in fuel cells. There are a number of areas of common interest to both programs such as corrosion, solid electrolytes for fuel cells, welding and joining, erosion, synthesis and processing of metals and ceramics, corrosion and heat resistant aluminides, and non-destructive evaluation. In a number of these programs it is clear that the fundamental understanding obtained basic scientific research helps in the solution of difficult technology development problems. The improvement of program integration activities helps increase the number of such linkages between science and technology. Further meetings are planned in order to isolate those areas where continuing interaction is most needed.

Dow Chemical Program Joint Review

Dr. John N. Mundy of the Office of Basic Energy Sciences/Division of Materials Sciences was an invited participant in a review of Dow Chemicals research contract under the Office of Industrial Technology/Energy Efficiency and Renewable Resources. Their contract is concerned with the development of continuous fiber ceramic composites based upon silicon nitride and aluminum nitride.

New Area of Commercial Application Explored for Non-Imaging Optics

In another example of technological applications of BES/Engineering Research-supported theory and practice of non-imaging optics, the Sacramento Municipal Utility Districts (SMUD) and National Renewable Energy Laboratory held a workshop in November on the potential use of solar thermal collectors in air conditioning (A/C). The workshop and the follow-on demonstration project are supported by Energy Efficiency, Office of Building Technologies. The object is to use absorption cooling (as is done in the well-known servel process) instead of electricity for air conditioning in local commercial and light industrial buildings. Absorption cooling requires a source of heat, and it is known that solar energy can serve as such a source. SMUD is reportedly willing to pay for the conversion of the existing A/C equipment in order to reduce peak loads, and hence postpone the need to expand electrical power generating capacity.

Interagency and International Cooperation

The Basic Energy Sciences programs have some substantial working relationships with other government agencies and international organizations to coordinate and interface program activities. Some examples of specific interactions are listed here.

Joint Meeting of the Steering Committees for the U.S.-Japan Cooperative Program on Neutron Scattering

The Department of Energy/Institute for Solid State Physics and the Department of Energy/Japan Atomic Energy Research Institute Steering Committees for the U.S.-Japan Cooperative Program on Neutron Scattering met at Brookhaven National Laboratory on June 2 and 3, 1993. In attendance were Drs. J. D. Axe, M. Blume, and M. Brooks from Brookhaven National Laboratory; Drs. R. Moon and R. Nicklow from Oak Ridge National Laboratory; Professors Y. Fujii and Y. Endoh from the University of Tokyo Institute for Solid State Physics; Drs. S. Funahashi and Y. Morii from the Japan Atomic Energy Research Institute; and Dr. I. L. Thomas from the Division of Materials Sciences/Office of Basic Energy Sciences at the Department of Energy.

The preceding year was again successful with 15 papers published or in press. The attendees were all disappointed that the High Flux Beam Reactor was not operating but pleased that the JRR-3M research reactor in Tokai, Japan, has operated for its full planned schedule of 28 weeks. The Japan Atomic Energy Research Institute has committed 100 million Yen for the upgrade of the WAND instrument at the High Flux Isotope Reactor. The status of the neutron scattering group at the Institute for Solid State Physics has been elevated to that of the Neutron Scattering Laboratory. The Institute is planning to build at Tokai an office and residence building for the Neutron Scattering Laboratory and visiting scientists. There was extensive discussion of the modifications that might be necessary to the existing arrangement to allow for a two-way exchange. Dr. R. Moon will prepare suggested modifications, and these modifications will be sent to Drs. S. Funahashi and I. Thomas. The intent is to begin the formal two-way exchange in 1994. The next meeting of the Joint Steering Committees will be hosted by the Japan Atomic Energy Research Institute in May or June of 1994.

Japan Expresses Interest in Establishing New Accelerator Facilities

An Oak Ridge National Laboratory scientist supported by the Office of Basic Energy Sciences/Division of Chemical Sciences attended a meeting in Japan and has reported that Japan's Science and Technology Agency is considering establishing a research facility based on the broad use of muon and radioactive ion beams. He recently visited Japan, sponsored by Japan, to present his ideas on the use of such beams for atomic physics research. Other presenters discussed the utility of the futuristic facility for research in nuclear, solid state, surface and medical physics. The ideas were exchanged among a group of 43 scientists, 12 non-Japanese (4 U.S., 3 German, 2 Russian and one each from France, Belgium and Sweden). At present, the Japanese are constructing a $400 million facility at the National Institute of Radiological Sciences that will have a capability comparable to that of the Bevalac. Japanese medical physicists will use the facility for heavy ion cancer therapy. The Japanese also are considering using muons and radioactive ion beams for therapeutic purposes.

Army Meeting on Light-Weight Materials for Dual-Use Technologies

Dr. Joseph B. Darby, Jr., of the Office of Basic Energy Sciences/Materials Sciences Division staff, was an invited participant at an Army Materials Research Conference that is concerned with the application of light weight materials (such as aluminum, magnesium, titanium and their respective alloys) through the week of September 3, 1993. This meeting is under the auspices of Technology Reinvestment Project to execute programs under the Defense Conversion, Reinvestment, and Transition Assistance Act of 1993, and thereby pursue dual-use technologies. The United States Army has been pursuing the application of such light-weight alloys for applications in tanks and other forms of armored vehicles. By replacing the conventional materials used in such vehicles with light-weight alloys which have a superior strength to weight and elastic stiffness to density ratios, it would be possible to achieve the necessary structural integrity yet decrease the weight of these vehicles, and thereby increase their fuel economy. Past and continuing government research efforts to improve the faricability, weldability, and behavior of such light-weight alloys could lead to their usage in both military and civilian ground surface vehicles. The Materials Sciences program has in-place expertise and laboratory and human resources that are in a position to make a contribution to this effort by the United States Army, which is why they invited Dr. Darby to be a participant in this meeting.

Meeting of the Committee on Materials Task Group on Structural Ceramics

The Federal Coordinating Council on Science, Engineering and Technology-Committee on Materials Task Group on Structural Ceramics, which consisted of 21 Federal program offices, including 7 from the Department of Energy, held a meeting on May 13, 1993.

The aggregate sums of nonclassified Federal, Department of Energy, and Office of Basic Energy Sciences research in structural ceramics are as follows:

(Funding in $M)	FY 1992	FY 1993	President's Request FY 1994
Total Federal	126.8	142.9	143.4
Total DOE	50.9	50.0	51.1
BES	7.7	8.2	8.2

The focus of this task group was on structural ceramics for mechanical load bearing applications at temperatures above 1000 degrees Celsius. The above funding survey is, therefore, restricted to such applications and does not include structural ceramics that are intended for lower temperature applications, such as transformation toughened zirconia and glass matrix composites or superconducting, solid electrolyte, refractory, dielectric, electro-optic, piezoelectric, nuclear fuel or neutron moderating ceramics, etc. The principal applications for structural ceramics above 1000 degrees Celsius are in various turbine and other propulsion system components and high speed cutting tools. Although heat exchangers are not normally subject to significant mechanical loading, the structural ceramic silicon carbide is becoming increasingly popular for such applications because of its good thermal conductivity and thermal shock resistance, as well as good fracture toughness that will permit it to tolerate impact accidents and erosion. Therefore, silicon carbide heat exchanger activities are included in our survey.

The agenda for this meeting focussed on matters of interagency communication and coordination of federally funded research in structural ceramics, and ways to sustain and enhance interactions with industrial structural ceramic suppliers and users. Dr. Charles Sorrell of the Department of Energy/Energy Efficiency and Renewable Resources/Office of Industrial Technology made a presentation on the developing National Advanced Materials Program Plan. Dr. Alan Dragoo of the Office of Basic Energy Sciences/Division of Materials Sciences made a presentation on Japanese research in structural ceramics. The Committee on Materials Task Group on Structural Ceramics was chaired by Dr. Robert Gottschall from the Office of Basic Energy Sciences/Division of Materials Sciences.

Three Agencies Meet on Plant Science Collaborative Research

On Saturday, April 17, 1993, a meeting was held at the Department of Agriculture in Washington, D.C., of the 13 representatives of the projects on multidisciplinary training and research coordination networks initiated in 1992 as part of the Department of Energy (Office of Basic Energy Sciences/Division of Energy Biosciences)/National Science Foundation/Department of Agriculture cooperative program on plant sciences. The objective of the meeting was to elicit information about progress being made and introduce the representatives so that exchanges and collaborations may be started. Along with an overview of the content and progress being made in each of the projects, various ideas emerged that may serve to enhance the value of the efforts. Overall, the collaborative program appears to be serving a very useful purpose by avoiding duplication of efforts, allowing the implementation of research that would not be especially feasible with individual grants, as well as encouraging greater interactions among investigators and institutions.

Twenty-Fourth Federally Employed Women's National Training Program

Cynthia Carter of the Office of Basic Energy Sciences/Division of Advanced Energy Projects, participated in five workshops during the 24th Federally Employed Women's Training Program held in Las Vegas, July 26-30, 1993. The program offered a wide range of topics with superbly-qualified instructors to help participants develop their work skills in areas ranging from work force diversity, team-building, and understanding of collaboration among different personalities, to skills in oral presentations, career building, and dealing with barriers in the way of potential achievements. The program was attended by more than 3,000 participants. While most were women of a wide range of diversities and grade levels, a number of men participated as well. A congenial tone prevailed at each workshop, encouraging all participants to engage in workshop discussions and practice sessions.

Review Conducted of Actinide Research in the Former Soviet Union

The DOE Office of Basic Energy Sciences has been essentially the sole support for the program of the production of the heavy (actinide) elements and the basic research on these nuclear materials in the United States. While this has been an outstanding program since the Manhattan Project, other countries have mounted very high quality programs, most notably the Soviet Union. The severe economic stringencies there have likely impacted major government programs in this area of science and materials production so it was chosen for review through the Office of Program Analysis. Science Applications International, Incorporated, was selected to pursue the review. They sent a review team of US experts to visit critical laboratories and production facilities in the Former Soviet Union for an on-site update of this important area of scientific research. An assessment of the status of heavy element science is available in a final report; contact Dr. John Burnett at (301) 903-5802).

International Energy Agency (IEA) Annex Meeting Focuses on Multiphase Flow Research

Dr. Oscar Manley of the BES/Engineering Research Program gave an invited talk at the IEA Annex meeting held in Bergen, Norway, December 8-10, 1992. With the depletion of the most productive oil and gas fields in the North Sea, IEA has shown an increasing interest in those aspects of multiphase flow research which bear critically on the economic exploitation of the lesser fields in that area. Dr. Manley briefed members of the Annex on the relevant basic research activities supported by his program, which focused on the transport of mixtures of oil, gas, and water in pipelines and in porous media. There were also presentations by representatives of DOE-Pittsburgh Energy Technology Center, University of Saskatchewan (Canada), Imperial College (United Kingdom), and Technion (Israel), as well as by Norwegian and Swedish researchers.

International Collaboration Seeks Improved Actinide Sequestering Agents

An investigator at the University of California/Lawrence Berkeley Laboratory, with support from the Chemical Sciences Division and in cooperation with the Commission of the European Community and the British National Radiological Protection Board, is developing protocols for the chemical removal of plutonium and other actinides from the body. Professor Ken Raymond has discovered non-toxic chemical agents derived from hydroxpyridone (HOPO) that effectively sequester plutonium and other actinides from body fluids. The sequestering agent containing the actinide contaminant is then excreted which prevents inclusion of the actinides in body tissue. The European collaborators who work in the European Late Effects Task Group, a group that studies the carcinogenic effects of actinide poisoning, have found that the HOPO derivatives are up to 30-times more effective in removing the contaminant than the currently accepted agent, diethylenetriaminepenta-acetic acid.

The Other DOE Provides Assistance to the DOE

A \$3.9 million grant from the U.S. Department of Education was awarded on November 4, 1992, to the University of Illinois toward the construction of a four-story building that will bridge the Materials Research Laboratory and the Coordinated Science Laboratory Buildings. The addition will provide much needed laboratories and office space for Materials programs funded by the U.S. Department of Energy and the National Science Foundation and will link the two buildings in which the Department of Energy funded programs are performed. The grant included a key provision that the money be used for "provision of facilities for advanced skill-training programs that relate to emerging technologies and skill needs." The Center for Microanalysis, a part of the Department of Energy funded Materials Research program, will occupy most of the new laboratory space.

North Atlantic Treaty Organization (NATO) 1993 Advanced Study Institute - Supercritical Fluids

Five of the fifteen plenary lecturers for the NATO Advanced Study Institute for Supercritical Fluids, Fundamentals for Applications, which was held in Turkey in July 1993, are supported by the Office of Basic Energy Sciences/Chemical Sciences Division. They are Professors Peter T. Cummings and John P. O'Connell at the University of Virginia, A. Z. Panagiotopoulos at Cornell, Stanley I. Sandler at the University of Delaware, and Jan V. Sengers at the University of Maryland. All of these have been previously recognized for awards or scientific contributions.

The objectives of the NATO institute are to review the current state of scientific knowledge on experimental and theoretical methods in the field, and to submit current measurement and modeling practices to critical examination. The technical program consists of core lectures and the plenary lecturers from an international community of supercritical fluids researchers.

NATO 1993 Advanced Study Institute—Nanophase Materials

This Advanced Study Institute was held in Corfu, Greece, on June 20 through July 2, 1993. The Institute was an intensive, two-week course on synthesis, properties, and applications of nanophase materials. The format of the course consisted of one hour lectures followed by several one-half hour talks on the subject of the lecture. Materials made from crystals that are 1-10 billionth of a meter in size are called nanophase materials. Because of the small size of the crystals, nanophase materials have interesting and, in some cases, unique properties. Some of the properties of particular interest to the Department of Energy include lower temperature sintering of ceramics, superplastic forming of ceramics and metals, higher strength magnets, and improved catalysts and catalyst support materials.

This Institute was unusual in that a wide range of disciplines was needed to cover the diversity of the topic. Lecturers included organic and inorganic chemists; experimental physicists; theoretical physicists and chemists; chemical, metallurgical, and ceramic engineers; and biologists. There were a total of 130 participants. All of the North Atlantic Treaty Organization countries were represented. Mexico, Canada, Russia, Bulgaria, Poland, and Hungary were also represented. United States industry was represented with people from Exxon, Xerox, duPont, International Business Machines, and American Telephone and Telegraph. The co-chairmen and several of the lecturers and speakers are supported by the Office of Basic Energy Sciences/Division of Materials Sciences which was represented by Dr. Iran Thomas. Although much good work was presented by the non-United States participants, the United States has a substantial lead in research; and judging from conversations with the industrial people, the lead is not just in research but also in applications.

Engineering Deans Meet with NSF, DOE

The Engineering Deans Group, an informal group of 14 deans from major U.S. research universities, met at the University of Maryland to discuss engineering research funded by NSF and DOE. Presentations were made by Joe Bordogna, NSF Assistant Director of Engineering, and Jim Coleman, Division Director for Engineering and Geosciences in the Office of Basic Energy Sciences. The discussions focused largely on funding prospects, trends and uncertainties related to the change in administrations. The chairman, Dean John A. White of Georgia Tech, stressed their willingness as a group or individually to provide any help they could give in support of the NSF and DOE engineering research efforts.

International Workshop on Ordered Intermetallics - Hangzhou, China

An International Workshop on Ordered Intermetallics was held on September 28, 1992 to October 1, 1992, in Hangzhou, China. The workshop was organized by Professor Dongliang Lin of Shanghai Jiao Tong University, and Dr. C. T. Liu of Oak Ridge National Laboratory, and sponsored by the National Natural Science Foundation of China. The participants included 17 foreign scientists, 30 Chinese scientists and 13 scientists from the United States, 7 of whom received funding from the U.S. Department of Energy.

The Chinese scientists have a large scientific effort on intermetallic materials and are anxious to interact with the world community. It appeared that about 80 percent of the work presented represented "catch-up" research and 20 percent was new and original research. They have good research facilities acquired through a World Bank Loan and they are performing quality research in this area. Dr. Joseph B. Darby, Jr., of the Division of Materials Sciences was an invited participant to give a talk on the U.S. Department of Energy programs on ordered intermetallics.

Third Continental Scientific Drilling Forum

The Continental Scientific Drilling Forum sponsored jointly by DOE, NSF, and USGS was held on October 26, 1992, in conjunction with the national meeting of the Geological Society of America in Cincinnati. The Forum was presented with updates on pending projects and projects-in-progress by ten different groups including the Katmai drilling project in Alaska, the hydrothermal mineral system of the Creede Caldera in Colorado, and the Triassic climatological and palaeomagnetic record of the Newark Basin. In addition, the Forum was presented with new concepts and developing projects in continental scientific drilling by 6 new groups. Among those projects presented for scientific nurturing and drilling strategy development, the proposed project in the Chicxulub Impact Crater stirred the most interest. Dr. James Coleman, Bill Luth and Tom Torgersen represented the BES/ Geosciences program at the meeting.

The Chicxulub Impact Crater in northern Yucatan represents the prime candidate for the Cretaceous/Tertiary boundary (65 Myr) event which includes mass extinction and the demise of most dinosaurs (*Nature*, October 29, 1992, vol. 359, pp. 819-821). Although the crater has no obvious surface expression, its typical crater structure is well defined by the gravity data. Wells drilled by the Mexican petroleum company (PEMEX) in the region show the melted rock, polymict breccias, shock metamorphism and high iridium that is expected. The size of the impact crater (210 km) suggests structural uplift of 20 km bringing the mantle boundary to within the range of deep drilling technology. A consortium is being brought together with scientists in the US, Canada, Europe and Mexico as well as PEMEX and AMOCO. The drilling project is sufficiently developed that drilling could begin as early as Spring 1993, contingent upon funding. The presentation of this project to the Forum represents a major step in the expansion of scientific drilling to a program of major international scientific collaboration.

Scientific Drilling Activities in Conjunction with the American Geophysical Union Meeting

In Conjunction with the American Geophysical Union (AGU) Meeting in San Francisco, December 7-11, 1992, several topical workshops were held at which BES/Geosciences research results were discussed. On December 5, two separate meetings were held; one dealing with the proposed shallow drilling in the volcanic sequence near Hilo, Hawaii, and one dealing with research results from the Creede, Colorado, shallow drilling of caldera fill sediments, both of which involve BES/Geosciences researchers. On December 6, a workshop was held at Menlo Park, California, where recent results of surface-based studies and proposed drilling at Katmai National Park, Alaska, were discussed. During the evening of December 8, a meeting was held on a proposed science plan for deepening a 2.5km deep hole at Long Valley, California. A workshop of over 100 participants at the Asilomar Conference Center, Pacific Grove, California, from December 13-16 focused on scientific drilling through an active tectonic-seismic zone, the San Andreas Fault in California.

Organisation for Economic Cooperation and Development (OECD) Megascience Forum: Expert Meeting on Geoscience Drilling

A meeting was held in Brest, France, on November 2-4, 1992, to gather information on the status and prospects of ocean and continental deep scientific drilling as a possible Megascience Program which could benefit from international collaboration at an early stage. A Megascience Program is contrasted with a Megascience Project, such as the SSC, in that it is not critically linked to a particular facility. The meeting was chaired by Dr. Tindemans (Netherlands), President of the Megascience Forum with support from the OECD Secretariat. Data was collected on the existing U.S., Canadian, French, German, Russian continental programs as well as on proposed activities in several other countries. The current contributors to the International Ocean Drilling Program (United States, Canada, Australia, Germany, France, Japan, United Kingdom, Belgium, Denmark, Finland Greece, Iceland, Italy, Netherlands, Norway Spain, Sweden, Switzerland and Turkey) were well represented in the presentations. Prof. Mark Zoback (Stanford University), provided the keynote scientific address. The U.S. delegation included the representatives of both the Continental (Dr. Ian MacGregor, NSF, Dr. William Luth, DOE/BES, and Dr. David Russ, USGS) and Ocean (Dr. Donald Heinrichs, NSF) Programs.

The current level of international expenditures for scientific drilling (deep and shallow), approximately $100 million per year, is at the lower margin for consideration as a Megascience Program. However, the participants agreed that international cooperation and collaboration was desirable to obtain maximum scientific benefit. Models for cost-sharing among Nations were not discussed except in individual conversations. Several researchers noted emphatically that "deep" has many different meanings and should not be thought of in terms of specific depth range of drill-holes. The important measure of depth is in terms of added depth of insight relative to processes taking place in the earth.

A wide range of frontier scientific drilling opportunities were presented. Of particular interest to the U.S. delegation were the Katmai shallow volcanic system (AK), San Andreas fault (CA), and the Chicxulub impact structure (Mexico). Each represents a unique opportunity to test and refine hypotheses based on indirect observation through in situ observations and experiments. Indeed, this was the theme of the meeting: a vital need to test hypotheses by direct observation. Direct access to the interior of the earth requires drilling, sampling, and in situ experiments. This same method of direct access is also the basis for use of our mineral, energy, and water resources.

The Expert Meeting provided input for two summary papers, in preparation by Prof. Carl Fuchs from Karlsruhe Universitat (Continental) and M. Pezard from the French Oceanographic Institute at Marseille (Ocean). These summary papers were integrated and summarized in turn by the OECD Secretariat as a report to the Megascience Forum Meeting in January 1993 (see below). The meeting was valuable since it provided an opportunity for interaction with representatives from other countries. The U.S. delegation established several new contacts and renewed some previous ones. Plans are to increase coordination with our Mexican and Canadian counterparts.

OECD Meeting on International Collaboration on Deep Drilling

The meeting of the Organization for Economic Cooperation and Development (OECD) Megascience forum on January 12-13, 1993, in Paris, France, considered scientific opportunities in astronomy and deep drilling. Dr. James Decker attended as the DOE representative. A technical meeting was held in Brest, France, November 2-4, 1992, to prepare background information on the current and future scientific orientation and challenges of deep drilling in the context of geosciences research and to evaluate existing mechanisms for coordination and cooperation. Dr. W. C. Luth, Office of Basic Energy Sciences, attended the technical meeting.

The Ocean Drilling Program is international in scope and thrust, with the United States being the lead partner. In the scientific community, there has been growing recognition of the need for internationalizing the scope and thrust of the continental counterpart. The need was clearly recognized at the 6th International Symposium on the Observation of the Continental Crust through Drilling (Paris, France, April, 1992), and in turn led to the proposition for an international scientific meeting on frontier challenges in the geosciences which could be substantively addressed by drilling. This meeting was held in August 1993, at Postdam, Germany, under the auspices of the International Lithosphere Program of the International Union of Geodesy and Geophysics. The 7th International Symposium will be sponsored by the U.S. Continental Scientific Drilling Program at Santa Fe, NM, in May, 1994.

The U.S. program currently involves the U.S. Geological Survey (DOI), the National Science Foundation, and DOE. It is coordinated by an Interagency Coordinating Group for Continental Scientific Drilling with participants from the three respective agencies: Dr. D. P. Russ, Dr. Ian MacGregor, and Dr. W. C. Luth (BES).

Advisory Council Reviews Triagency Continental Scientific Drilling

The Council for Continental Scientific Drilling is chartered under the Federal Advisory Committee Act to provide annual oversight of the U.S. Continental Scientific Drilling Program as conducted under the 1984 Accord entered into by the U.S. Geological Survey, National Science Foundation, and the Department of Energy. The Council met January 28 and 29, 1993, at the Forrestal Building. The three participating agencies devoted about $8 million to the Continental Scientific Drilling Program in FY 1992 and nearly $75 million over FY 1985 through FY 1992. At the meeting achievements were outlined resulting from drilling efforts at the Newark Basin (New Jersey), the Western Interior Seaway (Colorado), Manson Impact Structure (Iowa), Long Valley (California), and Creede (Colorado). Pending projects at Hawaii and Katmai National Park (Arkansas) were reviewed in terms of surface based pre-drilling research. Potential projects in the Florida Bahamas Banks, the Chicxulub Impact Structure in Yucatan, the San Andreas Fault (California), and at White Island, New Zealand were discussed as well as highlights from recent international meetings. The Council prepared a working version of its report prior to adjourning on January 29.

Interagency Geoscience Program in Continental Dynamics Research Initiated

A new Memorandum Of Understanding (MOU) to establish a somewhat broader role for the current Interagency Coordinating Group (ICG) for Continental Scientific Drilling (CSD) was discussed in detail at the ICG meeting of April 21, 1993. The existing MOU, "Interagency Accord on Continental Scientific Drilling," was approved in 1984 to implement interagency coordination provisions referenced in a joint Congressional Resolution of 1984 (P.L. 98-473) and extended in P.L. 100-441, "The Continental Scientific Drilling and Exploration Act." The new MOU, or Accord, will continue to fulfill the coordination provisions of P.L. 100-441, but will also be consistent with the emerging Interagency (National Science Foundation, United States Geological Survey, Department of Energy) theme where the Continental Scientific Drilling Program is included within a broader program of "Continental Dynamics." This change serves to emphasize that drilling, logging, sampling, and *in situ* experiments of the CSD are integrated with geophysical imaging, surface-based studies, experimental laboratory simulation and modeling, to gain a broader and more comprehensive understanding of processes and phenomena that affect the surface of the planet on which we live. The new "Interagency Accord on Continental Dynamics" will be prepared for signature by the Director of Energy Research for DOE, the Director of the National Science Foundation, and the Director of the U.S. Geological Survey for the Department of Interior as was the previous Accord.

The three agency participants in the CSD supported a workshop in 1989 which resulted in a recently published report entitled "Continental Dynamics" which delineates key elements of the broader program. Copies are available from W.C. Luth, Office of Basic Energy Sciences/Division of Engineering and Geosciences, ER-15, (3-5822) for distribution.

Advances in Continental Scientific Drilling Described

Dr. R. A. Kerr described important advances made by the German Continental Scientific Drilling Program in an (7/16/93) of *Science* (p.295-297). He noted the total expenditures of a third of a billion U.S. dollars in the German program to a obtain the 7.5km drill hole. U.S. researchers supported by the U.S. Geological Survey, the National Science Foundation, and the Department of Energy/Office of Basic Energy Sciences have participated in the scientific planning and research in this project from the outset under the auspices of the U.S. Interagency Coordinating Group for Continental Scientific Drilling.

Dr. Al Duba, of Lawrence Livermore National Laboratory, supported by the Office of Basic Energy Sciences/Geosciences program, was quoted and his research on the cause of the electrical conductivity anomaly at depth was a central point in the article. Consistent with other scientific drilling experiences here and abroad, the most important impact is in providing samples and measurements from depth that permit us to test our surface-based hypotheses and models. We continue to learn more about the earth's materials, the extent and nature of fluid flow in the earth's crust at depth, the causes for the geophysical anomalies and the origin of seismic reflectors through scientific drilling.

Kerr also refers to an upcoming meeting at Potsdam on international aspects of continental scientific drilling. This meeting will involve approximately 150 participants with 35 from the U.S. The scientific meeting at Potsdam will be followed by a meeting of program managers at the German Deep Drilling Site in Bavaria to identify ways and means for effective international collaboration in Scientific Drilling on the Continents.

Russian Geoscience Researchers at Lawrence Berkeley Laboratory

A program at Lawrence Berkeley Laboratory provided support for short-term (1-6 month) research in the Geosciences at Lawrence Berkeley Laboratory for Russian visitors during FY 1993. The program is complementary to one established by the Department of Energy's Office of Technology Development (EM-50) at Lawrence Berkeley Laboratory in that both emphasize transport of radionuclides at the Khystm (Chelyabinsk) site where a large release (2MCi) occurred in 1957. Visiting scientists brought knowledge of the existing database, recommendations for future data acquisition, and take advantage of existing modeling and geochemical capabilities at Lawrence Berkeley Laboratory. Transport data obtained from this large source can be of considerable value in assessing factors important in environmental restoration and nuclear waste disposal. It is also very important in fundamental geosciences because this large-scale "experiment" can provide a new class of information on transport and migration of geologic fluids bearing on a wide range of energy and environmental issues.

New Chair for Ocean Drilling Downhole Measurements Panel

Peter Lysne, of the Geosciences Research Drilling Office (GRDO) at Sandia National Laboratories, has accepted the nomination to serve as Chairman of the Downhole Measurements Panel of the International Ocean Drilling Program. The U.S. participation in the program is primarily through the National Science Foundation (NFS) and scientists supported by the NSF. The GRDO was established at Sandia in the mid 1980's to provide technological support for the DOE participation in the Interagency Continental Scientific Drilling Program. Contributions in this area from Sandia have proven to be of interest to the DOE's technology programs, to industry, and to the broader scientific community. The Downhole Measurements Panel is responsible for overseeing the implementation of sub-seafloor experiments. The panel receives information from the scientific community and uses this information to guide activities of the Borehole Research Group (Columbia, Lamont-Doherty Geological Observatory) and the Science Operations Group of the Ocean Drilling Program at Texas A&M. The panel is responsible for development of special instruments not provided by Schlumberger, the logging services contractor. Lysne has been very active in the GRDO and particularly in the development of down-hole gamma-ray logging techniques. He is now developing an improved fluid sampler for use in both the Oceanic and Continental Drilling Programs. As illustrated by this appointment, there is growing interest in scientific and technological collaboration in the Ocean Drilling Program and the Continental Scientific Drilling Program.

Technology Transfer Awards and Recognition

A primary goal of effective strategic research and development is the invention and use of new technology for the benefit of society. The processes by which this happens are not as simple as one might think. A common perception supposes a linear model of innovation, which assumes that scientists make discoveries, technologists apply the new knowledge, and engineers and designers turn the new applications into new products or processes. Unfortunately, like most simple models, people who study how science and technology interact believe that the linear model is an oversimplification and rarely exists in reality. Many times, those who deploy technology and those who benefit are genuinely unaware of, and perhaps uninterested in, the complex origins of the technologies which serve them. Given below are but a few examples of recent successes that were recognized.

Eight 1992 R&D 100 Awards Grow Out of Basic Energy Sciences-Supported Research

R&D Magazine annually issues 100 awards honoring innovation in industrial research. The October 1992 issue of the magazine, which features the R&D 100 Awards for 1992, highlights a BES/Division of Materials Sciences (DMS) program at the Pacific Northwest Laboratory (PNL) on its cover. The cover photo depicts the glycine-nitrate ceramic powder synthesis method developed by Drs. L. R. Pederson, L. A. Chick, and G. Exarhos of PNL. The project is one of 27 R&D 100 Awards which was sponsored by DOE national laboratories. The official award ceremony held at the Museum of Science and Industry in Chicago, Illinois, on September 24, 1992, was attended by Secretary of Energy James Watkins reflecting the strong role DOE has traditionally played in the program. In the 30 years the awards have been presented, DOE leads all federal agencies with a total of 301 winners. Although it is sometimes difficult to assess how well the R&D 100 Awards predict or influence commercial impact, a study of DOE winners from 1963 to 1988 revealed that 45% had been commercialized, with 17% having been licensed and 29 new companies were formed from these technologies. Indeed, many of the products selected for R&D 100 Awards have been major products for small, entrepreneurial companies that are key sources of innovation in U.S. industrial technology.

Eight R&D 100 Awards in 1992 are directly funded by BES or stem from BES-supported research. In several instances, the awards are excellent examples of the collaboration and cooperation between BES researchers and those of the other DOE basic and applied programs. Given below are brief descriptions of the eight BES-related R&D 100 Awards to illustrate how new knowledge gained through fundamental research may be used to advance technological innovation.

1992 R&D 100 Award: Adjustable Phase Undulator (APU-1)

An R&D 100 Award for 1992 was given to DMS-supported Roger Carr of the Stanford Synchrotron Radiation Laboratory scientific staff for the APU-1. The APU-1 is similar to a conventional permanent magnet undulator with a row of magnets above and a row below the electron beampipe. A conventional undulator's magnetic field is varied by changing the gap between the rows, but the APU's field is varied by changing the longitudinal position of one row with respect to the other. The effect on the x-ray spectrum is the same; it causes the characteristic energy of the x-rays to vary. But the effect on the electron beam of the APU-1 is less; there is much less change of horizontal steering and vertical focusing as the field is varied. Sensitive measurements of orbit perturbations showed no effect when the APU was scanned over the full range of its motion. This is important because it allows the APU-1 to be varied without disturbing other users of the storage ring. Also, the APU-1 is significantly simpler and about a fifth the cost of conventional systems, so it may be the design of choice for future undulators. APU-1 applications include lower cost sources for medical imaging, microscopy, spectroscopy, and lithography for semiconductor devices.

1992 R&D 100 Award: Gene Recognition and Assembly Internet Link (GRAIL)

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. Research on those techniques, supported by the BES/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 Oak Ridge National Laboratory. 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 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. Drs. Uberbacher, R. Mann, and R. Mural were honored with an R&D 100 Award this year for their accomplishments.

1992 R&D 100 Award: Pulsed Extraction Secondary Ion Mass Spectrometer

Research of Jim Delmore, Idaho National Engineering Laboratory, which has support from the Office of Health and Environmental Research, has been recognized with an R&D 100 Award for development of a new type of secondary ion mass spectrometer. Many materials--plastics, rubbers, ceramics, biopolymers, and paints--are not good electrical conductors and build up static charge during traditional spectroscopic analysis, making them difficult to analyze. But this system rapidly alternates the extraction of positive and negative ions at a rate of 20 times/sec to prevent the accumulation of static charge. The development of this technique has predicated on earlier research supported by the Division of Chemical Sciences in the Office of Basic Energy Sciences. Chemical Sciences supports jim Delmore's investigations of secondary ion mass spectrometry which has provided a better understanding of the fundamental interaction of ions with surfaces, the ion physics of these processes and the negative ion formation processes. The spectrometer that was recognized by the R&D 100 Award has found applications in areas of DOE technology development including the Office of Arms Control and Nonproliferation and the EM Office of Technology Development.

1992 R&D 100 Award: Ionization-Probe Printed-Circuit Board Head Gasket

The R&D 100 Award to Dr. Peter Witze at the Combustion Research Facility of Sandia National Laboratories/Albuquerque was for his development of an ionization-probe printed-circuit board head gasket for internal combustion engine research. Ionization probes installed in the head gasket of a spark ignition engine are used to measure the cycle-resolved arrival time of the flame at discrete points on the perimeter of the cylinder bore. Dr. Witze developed this device to aid in his own research where he has recently demonstrated that for a swirling flow fuel injection the location of the spark plug has virtually no effect on the combustion process. Although Dr. Witze's immediate research has been supported by the DOE Office of Conservation and Renewable Energy, the facility in which he has been able to conduct that research has been provided and supported by the Office of Basic Energy Sciences. In addition, his research has profited from his collaborations with BES-supported researchers at the Combustion Research Facility.

1992 R&D 100 Award: Solar Detoxification of Hazardous Organic Materials in Groundwater

Solar detoxification of organic pollutants by particulate semiconductors uses focussed sunlight directly to destroy hazardous substances in groundwater and industrial wastewater. The process, which requires a non-toxic catalyst, concentrates sunlight onto a clear tube. As wastewater passes through the tube, the sunlight causes a chemical reaction that destroys toxins. The R&D 100 Award-winning program on the photodecomposition of organic pollutants in aqueous waste streams by TiO_2 colloidal semiconductor particles is currently supported by the DOE Office of Conservation and Renewable Energy at the National Renewable Energy Laboratory and Sandia National Laboratories and is an outgrowth of BES/Chemical Sciences-supported research in solar photochemical energy conversion. The fundamental photoinduced charge separation processes in these systems have been delineated over the past 10-12 years by investigators in photoelectrochemistry in the BES program.

1992 R&D 100 Award: PRISM Software System

Polymer scientists traditionally blend existing polymers to create new materials. Development of these alloys has been limited by a lack of molecular design principles--beyond intuition--to guide the chemists. Dr. John Curro of Sandia National Laboratories/Albuquerque, Professor Kenneth S. Schweizer of the University of Illinois, and Mr. J. Dana Honeycutt of BIOSYM Technologies received an award for developing and commercializing a software system for prediction of thermodynamic quantities and phase equilibria for polymer blends. Initial work on the polymer statistical mechanics theory and calculational method termed the Polymer Reference Interaction Site Model (PRISM), was performed at Sandia National Laboratories/Albuquerque by Drs. John Curro and Ken Schweizer. Further work on the PRISM method by Dr. Ken Schweizer has been supported by the Department of Energy at the University of Illinois through the BES/Division of Materials Sciences. Dr. Schweizer has continued his collaboration with Dr. Curro at Sandia. Mr. J. D. Honeycutt of BIOSYM Technologies carried out the commercial development of the software program. The PRISM software system helps researchers by predicting properties of polymer blends from existing molecular structures and uses a statistical mechanics of polymer liquids to enhance existing theories.

1992 R&D 100 Award: Hard-Surfaced Polymers

Drs. Eal Lee, Monty Lewis, and Louis Mansur of the Oak Ridge National Laboratory (ORNL) received an award for a technique for hardening the surfaces of polymers using ion irradiation. The ORNL researchers developed a method for producing hard-surface polymers with high-energy ion beams as part of a BES/Materials Sciences funded program on modification of materials by irradiation. By using this technique the surface hardness of polymer such as polyimides can be increased up to 40 times. This processing improves polymer resistance to oxidation and chemical attach.

1992 R&D 100 Award: Glycine-Nitrate Process for Synthesizing Ceramic Powders

The glycine-nitrate ceramic powder synthesis method was discovered by Drs. L. R. Pederson, L. A. Chick, and G. Exarhos in a BES/Materials Sciences Program at the Pacific Northwest Laboratory. Further work on this method has been carried out by support from the Office of Fossil Energy for the development of lanthanum chromite powders for processing of ceramic ignitors. Here's how the process works: A homogeneous percursor solution of amino acide glycine and metal nitrates is mixed, combined with water, and heated to drive off the free water. The resulting viscous foam burns at temperatures up to 1450 C, forming ceramic ash particles of the desired oxide composition. The explosive effect of this synthesis is depicted on the cover of the October 1992 issue of *R&D Magazine*. The resulting ash has fewer carbon impurities and 30 times the specific gravity of powders produced by competing methods. The process has potential for making ceramic automotive engines, solid oxide fuel cells, and precise optical devices.

Five More R&D 100 Awards for 1993 are Associated with Basic Energy Sciences

The October 1993 issue of *R&D Magazine* featured the R&D 100 Awards for 1993. This year, the following five products growing from research supported by Basic Energy Sciences were among those honored:

*1993 R&D 100 Award: Omnidirectional Wheeled Platform**

One of the prestigious 1993 R&D 100 Awards for innovative engineering design goes to the Oak Ridge National Laboratory robotics researchers supported by the Basic Energy Sciences/Engineering Research program. It recognizes their invention of a novel ominidirectional wheeled platform, shown on the third inset photograph on the cover of this booklet.*

Mobile autonomous robots are often expected to carry out their tasks (e.g., inspection, maintenance, and repair) in constricted areas. Access to, and egress from such areas may be impossible using conventional wheeled or track platforms. Recently, members of the team at Oak Ridge National Laboratory-Center for Engineering Systems Advanced Research studying the scientific foundations for intelligent machines designed a novel, computer-controlled wheeled platform which permits simultaneous rotational and translational motion of the platform.

The resulting agility of the vehicle will permit it to extricate itself from tight spots inaccessible to other wheeled systems. The "wheels" in the novel systems are coupled pairs of truncated spheres, rather like fat tires mounted on a shaft so that they are freewheeling in the direction parallel to the shaft, while providing traction in the direction perpendicular to the shaft. The design calls for few parts, small wheel-wells, and provides smooth contact with the ground.

Beyond robotic applications, the new system is expected to be used in many other contexts, e.g., easier to maneuver wheelchairs for the handicapped, vacuum cleaners, factory-floor transport vehicles, and all-terrain vehicles.

1993 R&D 100 Award: Molecular Switch for Microcircuits

Innovation in miniaturization of electronic switches, pioneered by a research team headed by Michael R. Wasielewski of the Argonne National Laboratory, also won an R&D 100 Award. Dr. Wasielewski designed a molecule that acts as a picosecond electron switch when exposed to short pulses of visible light. This achievement opens up the possibility of developing molecular electronic devices based solely on electron motion within donor-acceptor complexes. 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 nanometers to an absorber at 546 nanometers. The work, which is being supported by the Division of Advanced Energy Projects/Basic Energy Sciences, grew out of basic research supported by the Division of Chemical Sciences.

1993 R&D 100 Award: Carbohydrate Protein Conjugates

Carbohydrate Protein Conjugates (CPCs) are used to stabilize proteins—enzymes and antibodies—in harsh environments, such as high temperatures or in organic solvents which may be found in industrial reactors. Enzymes are used as catalysts in chemical processes. Stabilizing them increases their lifetimes, which increases the efficiency of the processes. Typical CPC yields in enzymes are greater than 90%, compared to 1% for native enzymes under analogous chemical reaction conditions. Similarly, exposure of a CPC antibody (complexed with a pesticide) to an organic solvent did not affect its binding ability. In contrast, the corresponding native antibody completely lost its binding ability in a similar exposure.

The work was done both at Lawrence Berkeley Laboratory (LBL) and also at the Ohio State University. The LBL work was under the direction of Mark Bednarski and Mark Alper in the Center for Advanced Manterials (CAM) Enzymatic Synthesis of Materials (Biomolecular Materials) Program. Professor Matthew Callstrom was the collaborator in the Chemistry Department at the Ohio State University. The research that led to the development of this system was supported under a Work-for-Others contract by the Cargill Corporation. After the termination of the contract, research was continued as part of the BES-funded CAM Program. Throughout, the project was closely tied to other BES-funded research in the Enzymatic Synthesis of Materials Program.

1993 R&D 100 Award: Long Trace Profiler II

Precise measurement of large-radius optical components (such as the aspheric mirrors used to reflect x-rays) with conventional non-contact devices is both complex and prone to measurement error. The Long Trace Profiler II (LPT II) eliminates these problems by measuring parts 1 m or more in diameter using interference patterns from a laser beam split into two beams that are reflected off the sample surface as the probe traverses the sample.

The intrinsic low noise level of this system enables measurement of a 1-m-long surface with an error bar of only 3 nm. It also has the capability to measure the absolute curvature of surfaces, which means it does not need reference surfaces or calibration standards. The LTP II can detect flaws in mirrors used widely in synchrotron light sources, such as Brookhaven National Laboratory's (BNL) National Synchrotron Light Source, as well as in space telescopes, such as NASA's Hubble. The device represents a significant advance in absolute surface-figure measurement technology. It is so precise in measuring height errors on surfaces that it could accurately measure the diameter of a pencil lead at a fistance of five football fields.

Principal developers of the LTP II are Peter Takacs, BNL; Shi-Nan Qian, University of Science and Technology of China; and Steven Irick, LBL. An earlier version of the instrument was developed by Takacxs and Qian, in collaboration with Eugene Church of the Army's Research and Development Center. Brookhaven's development of the LTP II has been supported by BES's Materials Sciences Division. Continued development of the LTP II as a commmercial product is already underway through a CRADA between BNL and Continental Optical.

1993 R&D 100 Award: Processes for Making Phase-Pure Superconductors

Researchers at Argonne National Laboratory, supported by Energy Efficiency's Office of Utility Technologies, Advanced Utility Concepts Division, have come up with a fast and efficient method of producing commercial quantities of high-temperature superconductors with high purity and significantly improved properties. The process for making phase-pure superconductors provides better superconducting powders, in 10% of the time, at a temperature 200°F degrees lower, and at 40% of the cost, compared to current methods.

The phase-pure superconducting powders are obtained by heating a mixture of salts of the constituent chemical elements to 1470°F for 4 hours under reduced total pressure in flowing oxygen gas, followed by cooling in ambient-pressure oxygen. The mixed salts evolve gaseous species, including carbon dioxide, upon heating, and the dynamic vacuum in this process removes the evolved gases rapidly and efficiently.

Critical insight needed for the development of the process was gained from basic research supported by the Office of Basic Energy Sciences, Division of Materials Sciences. A collaborative effort between Argonne, Brookhaven National Laboratory, and Ames Laboratory (R. W. McCallum) discovered that the effective removal of carbon dioxide was essential for the formation of phase-pure superconducting powders. This crucial knowledge was utilized by Argonne's research team (U. Balachandran, J. E. Emerson, S. A. Johnson, and R. B. Peoppel) to design their award-winning process.

The ceramic superconductors produced by this process could someday find use in power generation, storage, and distributrion, and in magnets for magnetic resonance imaging (MRI). A private firm, Superconductive Components Inc., Columbus, OH, is selling the powders made using the technique.

American Chemical Society Award Given for Oil-Spill Cleanup Research

Professor Adam Heller of the University of Texas will receive the 1994 Award for Materials Chemistry, awarded by the American Chemical Society. This award, sponsored by the E.I du Pont de Nemours Co., is being given to Professor Heller for his research on oil-spill cleanup. Professor Heller's approach utilizes sunlight to photocatalytically reduce the oil to carbon dioxide and water. This is accomplished by sprinkling titanium dioxide beads on an oil spill. The oil coats the beads and the titanium dioxide acts as a photocatalyst. The nontoxic residue, which consists of sand-like particles, can be skimmed or allowed to float to shore. A company has been formed to develop and market the technology. Professor Heller will receive the award at the March 1994 National Meeting of the American Chemical Society in San Diego. The research to develop Professor Heller's process was supported by a grant from the Office of Basic Energy Sciences/Division of Advanced Energy Projects.

Basic Energy Sciences Researchers Win Federal Laboratory Consortium Technology Transfer Awards

The Federal Laboratory Consortium announced their Awards for Excellence in Technology Transfer. A total of 30 awards were made of which 12 are from the Department of Energy laboratories. Three of these twelve (25 percent) involve Office of Basic Energy Sciences programs:

1) Drs. L. A. Chick, L. R. Pederson, and G. J. Exarhos at Pacific Northwest Laboratory "for using a Cooperative Research and Development Agreement to revitalize a licensee's interest in commercializing the glycine nitrate process." The glycine-nitrate ceramic powder synthesis method was discovered in a Basic Energy Sciences/Materials Sciences program at Pacific Northwest Laboratory. Further work on this method has been carried out with support from the Office of Fossil Energy for the development of lanthanum chromite powders for processing of ceramic ignitors.

2) Drs. M. Bednarski and M. Callstrom at Lawrence Berkeley Laboratory "for the development of a new polymeric material which can significantly extend the active lifetime of enzymes and allow their use in harsh industrial environments."

3) Dr. E. S. Yeung at Ames Laboratory "for your devotion and efforts in transferring a new laser-based method for indirect fluorescence of biological samples." This award acknowledges his efforts to transfer specific fluorescence detector technology to the commercial sector. His initial work involved the development of a new laser-based fluorescence detector that permits quantitation of 10^{-10} molar concentrations in a 0.2 nL sample volume, which equates to approximately 3000 analyte molecules. This "Microfluor" fluorescence detector for

capillary separation techniques received an R&D 100 award in 1991 and it has been used to analyze the chemical contents of a single human blood cell. Other significant applications of this technology include environmental, industrial, and commercial separation processes.

Materials Sciences Principal Investigator is the 1993 Winner of the International Prize for New Materials

Dr. Gordon Osbourn of Sandia National Laboratories in Albuquerque, New Mexico has been selected as the winner of the American Physical Society's 1993 International Prize for New Materials for "originating the field of strained-layer superlattice electronics and optoelectronics by making the first theoretical calculations that predicted the unique electrical and optical properties of strained layer electronics and for inventing important new electronic and optical devices utilizing these properties."

Dr. Osbourn, who was funded at the time by the Department of Energy's Division of Material Sciences, predicted that useful new electrical and optical properties could be obtained by intentionally straining a combination of alternating layers of III-V compounds such as gallium arsenide, indium arsenide, and their alloys. His theoretical results directly motivated the first experimental studies of these new materials at Sandia National Laboratories/Albuquerque. The subsequent work of Dr. Osbourn and others at Sandia supported by the Office of Defense Programs, used individual and multiple strained layers which resulted in the development of the following device structures: 1) world-record high-frequency/low-noise indium gallium arsenide-based transistors; 2) tunable low-threshold indium gallium arsenide-based diode lasers and surface-emitting lasers; 3) wavelength tunable indium gallium arsenide-based optical modulators; and 4) long-wavelength III-V photovoltaic infrared detectors.

The useful electrical and optical properties of these materials, combined with their clearly established long-term stability in devices ranging from injection lasers to field effect transistors, continues to motivate materials and device applications in laboratories all over the world. Dr. Osbourn was awarded the Prize in Seattle during the March 1993 meeting of the American Physical Society.

Materials Scientist Receives Significant Honor/Facilitates Technology Transfer

Dr. Chain T. Liu, Group Leader in the Metals and Ceramics Division, Oak Ridge National Laboratory, has been elected a Fellow of The Minerals, Metals and Materials Society. The Fellows designation is limited to 100 living people at any time and three were elected for installation in 1994. It is, therefore, a restricted and significant honor. Dr. Liu has been the prime leader in the research on intermetallic materials for the Division of Materials Sciences, Office of Basic Energy Sciences, at Oak Ridge National Laboratory and has interacted with the American industrial community to bring their attention to the unique and useful potential for this family of materials.

This pioneering research on intermetallic alloys has directly or indirectly lead to eight License agreements and several Cooperative Research and Development Agreements with United States companies. Besides his Basic Energy Sciences effort, Department of Energy technology programs in the Offices of Energy Efficiency and Renewable Energy and Fossil Energy have provided support for the development of commercial and modified intermetallic alloys for industrial use in various energy and non-energy applications.

Dr. Liu has international recognition for his research and the organization of conferences and workshops in Europe through the North Atlantic Treaty Organization and in Asia through the Chinese National Science Foundation and the Japanese Ministry of Education, Science and Culture.

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Site Review Activities

Mechanisms to ensure that the Basic Energy Sciences program supports excellent quality research projects have always been an integral part of the program's funding processes. Each grant application proposal routinely undergoes external peer review and staff merit review, including relevance to Departmental missions. There are on-site reviews of ongoing research at the laboratories, contractor review meetings, and evaluation of research progress through the monitoring of reports, conference presentations, and refereed publications in scientific journals. An external audit of 744 individual Basic Energy Sciences research projects from May 1992 to November 1993 by the Office of Program Analysis proved that the program supports higher quality research projects than other Department of Energy programs assessed during the period 1983 - 1991. Examples of routine project reviews conducted by Basic Energy Sciences staff are given below.

<u>Reviews of Metallurgy and Ceramics Programs at Lawrence Livermore National Laboratory and Sandia National Laboratories</u>

Dr. Alan L. Dragoo of the Office of Basic Energy Sciences/Division of Materials Sciences conducted on-site reviews of the Division's Metallurgy and Ceramics programs at Lawrence Livermore National Laboratory and Sandia National Laboratories/California, on September 28 and 29, 1993. Discussions were held with program managers and presentations were made by laboratory staff engaged in Metallurgy and Ceramics programs. On-site reviews of material science programs at the National Laboratories are conducted on an annual basis by staff of the Division of Materials Sciences.

<u>Geophysics Workshop Concludes Four-Session Geosciences Series</u>

A Geophysics Workshop was held September 10-11, 1993, at the M.I.T. Endicott House in Dedham, MA, to provide a forum for exchange among university and laboratory researchers supported by the Office of Basic Energy Sciences/Geosciences Research Program. The workshop was hosted by Professor Toksoz of M.I.T. and included twenty-nine presentations covering current research of forty investigators and co-investigators. The topics included seismology, electromagnetic imaging, modeling of geophysical phenomena, and computational analysis of observational geophysical data. Copies of the Abstracts and the meeting agenda are available from the BES Division of Engineering and Geosciences.

This workshop concluded a series of four in the Geosciences during 1993. Previous workshops were at Caltech in January (Geochemistry and Mineralogy), at Sandia in May (Rock Mechanics and Continental Drilling), and at Berkeley in July (Aqueous and Organic Geochemistry) which covered all active and recently active projects in the program.

<u>Division of Materials Sciences Staff Conducts Program Review at the University of Illinois</u>

The Seitz Materials Research Laboratory at the University of Illinois has forty-four programs funded by the Office of Basic Energy Sciences/Division of Materials Sciences, at an annual level of six and a quarter million dollars. The programs cover various aspects of bulk, surface and thin film behavior of metals, semiconductors, superconductors, ceramics, polymers, and corrosion. Drs. Joseph B. Darby Jr., and John N. Mundy reviewed the science carried out under support from our Metals and Ceramics Branch and Mr. Michael F. Teresinski reviewed environmental and safety aspects of the program, on September 10, 1993, in Urbana, Illinois.

The Continuous Fiber Ceramic Composites Program Review Held in Washington

The review was held by the Department of Energy to introduce and discuss the industrial application of Continuous Fiber Ceramic Composites. These materials are both lightweight and corrosion resistant, and together with their high temperature strength show promise for use in a number of industrial technologies such as turbines and chemical reformers. The review was attended by over two hundred people representing industry, university and government laboratories. The majority of the speakers represented industries with research and development programs with Continuous Fiber Ceramic Composites and it was clear that while they recognized and wanted government help with research and development in the area of Continuous Fiber Ceramic Composites, they were not reticent in suggesting the 'appropriate conditions' for that help. The format of the meeting, one large hall, and all prepared talks was not conducive to interaction and the large number of attendees demonstrated an interest which might be better served by a two day conference where many more specific technical problems could be discussed. Alan Dragoo and John Mundy from the Office of Basic Energy Sciences/Division of Materials Sciences attended the meeting as part of the Division's continuing effort to maintain an awareness of activities and possible research needs of the Department of Energy technology programs.

Peer Review at Ames National Laboratory

The Office of Basic Energy Sciences, Division of Chemical Sciences carried out its annual review of continuing research projects at Ames laboratory in May. Approximately one third of the research projects supported by the Chemical Sciences Division in each of the Processes and Techniques and Fundamental Interactions Branches were reviewed by an external peer review committee. The Chemical Sciences Division was represented by Drs. Stephen Butter and Clement Yonker. The external reviewers were Professor Jim Atwood from SUNY-Buffalo, Professor James Cox from Miami University, Dr. Joe Berkowitz from Argonne National Laboratory, Professor Nicholas Delgass from Purdue University, Professor John Lamb from Brigham Young University, and Professor Bob Ziff from the University of Michigan.

The reviews consisted of formal presentations of current research to the peer review committee by the investigators, informal laboratory visits and discussions with the principal investigators, and executive sessions for preliminary oral reports followed by written reports from each reviewer. Topics for review during this session included interfacial chemistry and structures, ion separations, surface catalysis and theory, quantum chemistry, and the chemical physics of organosulfur compounds. These projects involve basic research relevant to various technology development programs of the Department of Energy.

Eleventh Symposium on Energy Engineering Sciences

The Eleventh Symposium on Energy Engineering Sciences was held at Argonne National Laboratory, May 3-5, 1993. Thirty-seven technical papers were presented, reflecting the activities of about one-third of the Office of Basic Energy Sciences/Engineering Research Program. Topics covered included various aspects of multiphase flows, elastic and inelastic behavior of materials, diagnostics, measurement techniques, and control of systems and processes. A highlight of the program was a group of papers dealing with flows of granular materials and rheology of dense suspensions. This fundamental research contributes to the understanding of such energy related processes as efficient pulverization of coal, transport of slurries, and handling of granular materials in mining operations as well as in industrial plants.

Chemical Sciences Programs Peer Reviewed at Oak Ridge National Laboratory

The Chemical Sciences Division carried out two annual reviews of research projects at ORNL in April. Approximately one half of the research projects supported by Chemical Sciences in each of the Chemistry and Analytical Chemistry Divisions were reviewed by two external peer review committees. The external reviewers for the Chemistry Division were Dr. Phillip Kleinschmidt from Los Alamos National Laboratory, Prof. Wilfred Tysoe of the University of Wisconsin-Milwaukee, and Dr. Richard Zepp from the U. S. Environmental Protection Agency Laboratory in Athens, Georgia. The reviewers for the Analytical Chemistry Division were Professor Jim Winefordner from the University of Florida, Professor Gary Horlick from the University of Alberta, and Dr. Jack Fassett from the National Institute of Standards and Technology.

The reviews consisted of formal presentations by the principal investigators of their current research, laboratory visits by the reviewers, and executive sessions by the peer review committees for preliminary oral reports followed by written reports from each reviewer. Topics for review during this session included analytical laser spectroscopy, inorganic mass spectrometry, photochemistry on surfaces, actinide chemistry, and surface catalysis. These research projects involve basic research relevant to the various technology development programs of the Department of Energy.

Reviews Held at the Notre Dame Radiation Laboratory

The annual review of chemistry programs at the Notre Dame Radiation Laboratory was held April 19-21, 1993. DOE was represented by Allan Laufer and Mary Gress of the Division of Chemical Sciences. The Visiting Committee for the research program consisted of Larry Kevan (Houston), Thomas Mallouk (Texas at Austin), Gary Schuster (Illinois), and Peter Wardman (Gray Laboratory, Middlesex, United Kingdom). The Committee was favorably impressed by the quality and breadth of programs, half of which are reviewed each year. The reviewers did, however, allude to the need for reorganization of the laboratory into larger groups with common goals when a new Director takes charge in the foreseeable future. The Data Center Advisory Board which met on April 21 was comprised of James Demas (Virginia), James Espenson (Ames Laboratory), Norman Klassen (National Research Council), and Peter Wagner (Michigan State). Jean Gallagher, representing the Standard Reference Data Program at National Institute of Standards and Technology which shares with DOE the support of the Data Center through an Interagency Agreement, was also in attendance. The Board advises on needed data compilations and dissemination mechanisms for data products.

Status of X-ray Optics for Synchrotron Light Sources

On October 28-29, 1992, approximately 40 scientists, primarily from the National Laboratories, met at Half Moon Bay, California, to discuss the status of X-ray optics research and development as related to the functioning and use of the synchrotron light sources. The workshop was chaired by Dr. James Underwood of the Lawrence Berkeley Laboratory, Center for X-ray Optics and sponsored by the Division of Materials Sciences, Office of Basic Energy Sciences. Participation included representatives from the National Synchrotron Light Source, the Advanced Light Source, the Advanced Photon Source, and the Stanford Synchrotron Radiation Laboratory.

Topics covered by the discussions were optics and concepts associated with polarization, high heat loads, multilayers, crystallography, metrology, microscopy/microprobing, and high resolution monochromators. A report summarizing the proceedings and conclusions of the workshop is being prepared and should be available within the next few months.

Science Policy Committee of the Stanford Linear Accelerator Center

The first meeting of the committee which advises on Stanford Synchrotron Radiation Laboratory and the remainder of Stanford Linear Accelerator Center was held April 9 and 10. Topics included the status and plans for the Synchrotron Radiation Laboratory as well as a report from the users group. The Linear Accelerator users group provided information to the committee and, in addition, there was an extended discussion about the B-factory program at the laboratory. John O'Fallon from High Energy Physics and Allan Laufer from Basic Energy Sciences represented the Department at the meeting. The advisory panel discussed the future opportunities for the laboratory in a very candid and open manner. The importance of appropriate technological use of the synchrotron facility by users who are local to the area, e.g., "Silicon Valley" manufacturers was stressed. The Committee reports to the President of Stanford University.

Chemical Sciences Division Programs at the Combustion Research Facility Reviewed

Programs in chemical dynamics and kinetics at the Combustion Research Facility, Sandia National Laboratories, California, were reviewed on March 22-25, 1993. Present for the review were representatives from the Division of Chemical Sciences, peer reviewers from Rice University, the University of California at Los Angeles, and SRI International, Inc.

The programs being reviewed were those efforts at the Combustion Research Facility concerned with the fundamental chemical processes that occur during combustion including the breaking of chemical bonds, the distribution of energy in reaction products, the rates of chemical reactions, and the analysis of complex processes in terms of their constituent chemical reactions and their reaction rates. Specific problems currently being emphasized include determination of the pathways for the formation of NO_2 and soot and on novel spectroscopic techniques applicable to combustion diagnostics. The reviewers were also given brief presentations on combustion related activities supported by other Department of Energy programs and were shown the Burner Engineering Research Laboratory, a joint effort between Department of Energy and the Gas Research Institute.

The reviewers commended the Combustion Research Facility on the overall excellence of its research efforts, its international reputation, and the international reputation of its staff. Recent promotions and other staff changes at the Combustion Research Facility have raised opportunities for shifts in research direction and the reviewers advised maintaining the balance between fundamental studies of chemical dynamics and more applied studies of combustion processes.

Chemical Sciences Division Review of Lawrence Berkeley Laboratory Research

A review of scientific programs supported by the Chemical Sciences Division was held at the Lawrence Berkeley Laboratory on March 1-3, 1993. The Chemical Sciences Division was represented by F. Dee Stevenson. The programs reviewed covered 1) new research on the synthesis of sequestering agents for plutonium ions, 2) carbon-hydrogen bond activation related to more energy efficient chemical conversions, 3) metal-ligand studies using steric barriers to kinetically hinder ligand rearrangement related to the problem of immobilizing waste materials in the environment, 4) synthesis of new functionalized polycyclic aromatics and organometallic chemicals with cyclopentadienyl ligands, some of which undergo interesting photochemical reactions relevant to energy storage, and 5) thermodynamic studies on modeling the behavior of polymers, studies of antisolvents for more energy efficient separations, and pioneering work on proteins.

The following reviewers assisted in the process: Herb Kaesz (University of California at Los Angeles), T. Alan Hatton (Massachusetts Institute of Technology), George Gokel (University of Miami), and Peter T. Wolczanski

(Cornell University). In a close-out session to be followed up with a formal report to the lab director, the reviewers were complimentary of the high quality of research, some world class, which seemed to be proceeding extremely well, and were generally well-focussed on Department of Energy missions.

Chemical Sciences Programs at Pacific Northwest Laboratory Reviewed

Experimental programs at the Molecular Sciences Research Center at Pacific Northwest Laboratory were reviewed on February 22-24. Present for the review were representatives from the Office of Basic Energy Sciences/Division of Chemical Sciences, and peer reviewers from Princeton University, the University of Utah, and the University of California at Berkeley. The programs being reviewed were those designed to provide fundamental knowledge about physical and chemical processes at surfaces that would affect the fate of chemicals introduced into soils and ground waters. Although much of the effort of this research group is aimed at the design of the new Environmental and Molecular Sciences Laboratory at Pacific Northwest Laboratory, a broad range of research is currently underway by the young staff that has recently been hired. The peer reviewers commended management for hiring truly excellent scientists and for identifying forefront research areas that were clearly relevant to the environmental problems facing Department of Energy. The reviewers criticized aspects of the infrastructure at Pacific Northwest Laboratory which they felt needed improvement. Pacific Northwest Laboratory management is aware of this problem and is taking steps to improve the responsiveness of the administrative services to the programmatic needs of the laboratory.

Tiger Team Corrective Action Followup Review Held at Oak Ridge National Laboratory (ORNL)

The ES&H staff members of the Chemical Sciences Division participated in the Tiger Team Corrective Action Followup Review of ORNL. The review was conducted the week of December 7-11, 1992, with a 15-member review team (ER, NE, EM) led by ER/ST-30. This was the first ER-led ES&H performance review of ORNL and occurred approximately one year after the approval of the Corrective Action Plan.

Radiation Effects Contractors Meeting

Twenty-three scientists participated in the BES/Materials Sciences Division Neutron Radiation Effects Contractors Meeting in Boston on December 1, 1992, including four scientists funded by the Office of Magnetic Fusion Energy. The major focus of this group is the coordination of research efforts and collaboration amongst various organizations. Collaborative research is especially desirable in order to achieve the maximum utilization of expensive and limited neutron irradiation time.

Chemical Sciences Programs at Argonne National Laboratory Reviewed

Programs supported by the Chemical Sciences Division of BES in both the Chemistry and Physics Division were reviewed between November 15 and November 20, 1992. Programs in combustion and coal science in the Chemistry Division and the atomic physics research program in the Physics Division were examined. Several external reviewers for each of the programs under review as well as representatives from the Chemical Science Division along with the appropriate division management heard presentations from representatives of the programs and had an opportunity for extensive, informal visits with all of the principal investigators in their offices and laboratories. The programs received strong technical endorsements from the reviewers who also recommended an increase in the number of postdoctoral positions. An important feature of this review is the participation of both DOE and laboratory management in the discussions of the merits of each of the programs.

Welding Science Research Discussed at Contractors Meeting

The annual Basic Energy Sciences/Materials Sciences Welding Science Contractors Meeting was held on October 8-9, 1992, at Pennsylvania State University. There were a total of 20 participants including some from universities, industry, Navy, and DOE laboratories that, while not funded by the Basic Energy Sciences program, are either collaborants or interactive with it. Principal scientific topics of discussion included weld-metal composition control, residual stresses, microsegregation during solidification, and fracture behavior of welds.

Aqueous Corrosion Research Discussed at Contractors Meeting

The annual Department of Energy (DOE) Aqueous Corrosion Contractors meeting was held on September 10-11, 1992, at the University of Illinois. Most of the 19 participants are funded by Basic Energy Sciences/Materials Sciences and amongst them 13 were from universities, and 5 from DOE laboratories. Topics of discussion included aspects of stress-corrosion, prediction of localized corrosion damage, mechano-chemical aspects of ultrasound, morphological aspects of anodic dissolution, adsorption of corrosion-active species by radioactive labeling, in-situ X-ray Absorption Near Edge Spectroscopy (XANES), studies of corrosion-passive films, in-situ X-ray scattering from electrode surfaces, surface-layer reconstruction, nonlinear optical characterization of surfaces, electron-transfer in corrosion systems, imaging atom probe analysis of a liquid-solid interface, radiation-induced segregation, hydride formation and fatigue crack growth, and atomic resolution electrochemistry. One of the non-DOE funded participants was from the Gas Research Institute. This group decided to meet again in Autumn 1993 with the Colorado School of Mines as host.

Basic Energy Sciences Advisory Committee (BESAC) Meets to Review Basic Energy Sciences (BES) Laboratory Programs

A BESAC meeting was held October 1, 1992, in Gaithersburg, Maryland. The full Committee reviewed BES program management and continued discussions with Brookhaven National Laboratory management. A status update of the Office of Program Analysis (OPA) Reviews of BES was also presented by OPA staff. The final BESAC report on the BES program at four major national laboratories (BNL, ORNL, LBL, ANL) was issued in September 1993.

Center for Engineering Systems Advanced Research (CESAR) Advisory Committee Review

ORNL's advisory committee for the Center for Engineering Systems Advanced Research (CESAR) conducted a 2-day review of CESAR's robotics and intelligent system program at ORNL during October 1-2, 1992. The purpose was to offer advice and guidance concerning major technical activities at CESAR including combined mobility and manipulation systems, multi-sensor data analysis and fusion, machine learning, behavior-based and hybrid robot control, and high performance computing environments. Among the highlights was a demonstration of the ability of a light-based sensor at the end of a redundant manipulator to remain a fixed distance from a curved surface as it moved along the surface. Both the manipulator arm and mobile platform on which it was mounted were programmed to move simultaneously. Drs. Oscar Manley and Daniel Frederick of the Office of Basic Energy Sciences/Engineering Research Program attended. The advisory committee, composed of 5 experts from U.S. universities, had many positive comments regarding the efforts at ORNL and their impact on the field of robotics.

Atomic Physics Contractor Meeting Held

The 13th annual meeting of all principal investigators, contractors and grantees, supported by the Basic Energy Sciences Atomic Physics Program was held at Cornell University on October 15 and 16, 1992. Invited guests included scientists supported by the Office of Fusion Energy. The group was welcomed by Dr. John Hopcroft, Associate Dean of the College of Engineering, 1986 winner of the Turing Award in Computer Science and new member of the National Science Board. During his remarks, he reiterated the importance of basic research to developing technologies and the need for the scientific community to provide a better justification for allocation of public resources for basic research. Other meeting highlights included reports on (1) pair production in collisions of high energy heavy ions followed by ion electron capture, a process relevant to modeling RHIC's ion beam integrity and (2) progress made in low temperature plasma physics relevant to the fabrication of microelectronic devices. A tour of Cornell's Electron Storage Ring revealed that a substantial effort has continued over the last three years toward its eventual submission of a competitive proposal for construction of a B-factory.

Review of Brookhaven Chemical Sciences Programs Held

Programs in the Departments of Applied Science (DAS) and Chemistry at Brookhaven National Laboratory were reviewed during the week of October 26, 1992, by a team of external, peer reviewers and members of the Chemical Sciences Division. Reviewed programs in DAS were in porphyrin chemistry, electrochemistry and the chemistry of hydrides while the complete radiation chemistry program in the Chemistry Department was examined. The reviewers were provided with background material, including relevant publications, before their arrival at the lab. The on-site review consisted of a formal presentation followed by intensive visits and discussions with the Principal Investigators in their laboratories. This will be a written report that summarizes the frank and candid discussions between the reviewers, laboratory management and DOE program representatives.

BES/ES&H Activities

ES&H staff specialists of the BES/Chemical Sciences Division participated in the Basic Energy Sciences User Facility Workshop held at Brookhaven National laboratory. Issues related to ES&H at the BES facilities were discussed. Some of the concerns discussed at the workshop which require BES attention are appropriate ES&H training needs for users, communication between facility personnel and users, electrical safety, and chemical handling.

BES continues its seminar program to educate staff on ES&H issues. For example, a seminar, presented by a member of the BES/Chemical Sciences Division, was entitled "Process Safety Management" and dealt primarily with the issue of accidental chemical release that could be a threat to employee health.

Other activities include ES&H staff participation in the Advanced Photon Source safety review and the evaluation of progress on the corrective Action Plan for the Tiger Team Assessment Report for the Princeton Plasma Physics Laboratory.

Materials Sciences Program Externally Reviewed at Ames Laboratory

Ames Laboratory conducted its annual review of the Materials Sciences Program at Ames on October 14-16, 1992. The review focussed on one-third of the projects supported by the BES/Division of Materials Sciences (DMS), and the external reviewers consisted of eight experts in metallurgy and ceramics, solid state physics, and materials chemistry. The reviewers were Alan Lawley - Drexel University, C. P. Flynn - University of Illinois, John Hren - North Carolina State University, Neal Shinn - Sandia National Laboratories/Albuquerque, Harris Marcus - University of Texas, Cliff Myers - State University of New York/Binghamton, Brian Maple - University of California - San Diego, and Douglas Mills - University of California/Irvine. The reviewers provided a verbal summary of their impressions to laboratory management at a close-out session following the formal presentations and visits by the reviewers with the principal investigators. A written report will be submitted to the Laboratory Director in a few weeks. Richard Kelley represented DMS at the review.

One of the highlights of the review was the presentation by C. T. Chan of the Condensed Matter Physics group of exciting new results on the theoretical prediction of the total energy, the equilibrium surface structure and stoichiometry, and the electronic properties of an overlayer of noble metal on a silicon single crystal (the (111) facet). This system has been intensively studied for 15 years - it is probably the most studied overlayer system in surface physics. It has also been among the most elusive and controversial surface system ever studied. The system and variants of it are important for the understanding of and the search for new electronic, solar, and photovoltaic materials. The first principles calculations by the Ames' Condensed Matter Physics group have predicted the detailed atomic level structure and energetics of this system. The theoretical predictions have been recently confirmed experimentally at several U.S. universities and at A&T Bell Laboratories. It appears that this problem has been solved. The theoretical techniques are currently being applied to other systems.

Seventeenth Solar Photochemistry Research Conference Held

The Seventeenth Department of Energy Solar Photochemistry Research Conference was held June 6-10, 1993, at Cragun's Conference Center in Brainerd, Minnesota. The annual meeting, sponsored by the Office of Basic Energy Sciences/Division of Chemical Sciences, was hosted this year by the Ames Laboratory. There were 109 participants in attendance, including 60 scientists from the Department of Energy's laboratories, 47 university grantees, and Mary Gress and Allan Laufer representing the Division of Chemical Sciences. Following brief welcoming remarks by Thomas Barton, Director of the Ames Laboratory, the program featured a guest plenary lecture by Graham Fleming, of the University of Chicago, on ultrafast spectroscopic studies of molecular dynamics in the condensed phase, 28 other formal presentations, and 58 posters. The research topics included: investigations on ultrafast (femtosecond time scale) phenomena in solution, electron transfer, and charge separation at interfaces; photosynthesis and molecular models thereof; photoinduced charge transfer in homogeneous and heterogeneous solutions; inorganic photochemistry; and photoelectrochemistry. Copies of the Proceedings are available from the Division of Chemical Sciences, (301) 903-5820.

Special Basic Energy Sciences Advisory Committee Panel on Neutron Sources

The Special Panel on Neutron Research and Sources established under the auspices of the Basic Energy Sciences Advisory Committee (BESAC) held a Workshop at Oak Brook, Illinois on September 6-8, 1992, to examine the needs of the nation in neutron science and the options available. The panel is chaired by Walter Kohn of the University of California at Santa Barbara. The panel has visited each of the major existing neutron sources at DOE laboratories. The workshop has the purpose of defining the technical options and opportunities, so that the panel can make recommendation to the Director of Energy Research with respect to the various options. The workshop included 70 participants from laboratories around the world in addition to the 12 panel members. The workshop was divided into working groups on neutron sources (Reactor Sources and Spallation Sources) and neutron applications (Condensed Matter Physics, Chemistry Polymers and Complex Fluids, Biology, and Materials Research, Isotopes, Materials Irradiation, Materials Analysis and Imaging, Positrons and Muons, and Fundamental Physics) in addition to a working group on Instrumentation. Professor Kohn expressed the Committee's recommendations to the Director of Energy Research by letter on September 15, 1992, and briefed the SEAB Townes Committee on September 24 in Washington, D.C. The full report, "Neutron Sources for America's Future," was issued in January 1993 and is available from the Office of Basic Energy Sciences, (301) 903-3081.

Plant Research Laboratory Reviewed by the Division of Energy Biosciences

The staff of the Division of Energy Biosciences, along with a group of six internationally recognized experts in the field of plant biological research, conducted an extensive site review of the Michigan State University/Department of Energy Plant Research Laboratory in September 1993. The thirteen principal investigators affiliated with the laboratory each made scientific presentations and answered questions. The graduate students, post-doctoral fellows, support staff and visiting scientists were also interviewed by the site reviewers. This comprehensive scientific review is routinely conducted every three years.

List of Titles

Technology Transfer Activities

Integration with U.S. Industry

Site Review Activities