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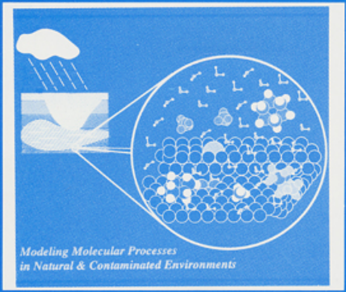
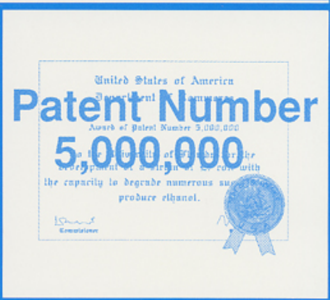
U.S. Department of Energy

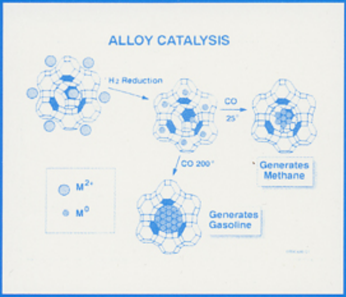
Office of Energy Research

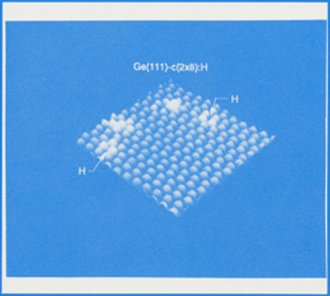
Office of Basic Energy Sciences

1991 Summary Report









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U.S. Department of Energy
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1991 Summary Report

A summary of the organization, mission, and activities of the Office of Basic Energy Sciences

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Washington, D.C. 20585

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Introduction

Basic research is an important investment in the future and will help the U.S. maintain and enhance its economic strength. The Office of Basic Energy Sciences (BES) basic research activities, carried out mainly in universities and Department of Energy (DOE) laboratories, are critical to the Nation's leadership in science, for training future scientists, and to fortify the Nation's foundations for social and economic well-being. Attainment of the national goals -- energy self-sufficiency, improved health and quality of life for all, economic growth, national security -- depends on both technological research achievements and the ability to exploit them rapidly. Basic research is a necessary element for technology development and economic growth.

This report presents the Department of Energy's Office of Basic Energy Sciences program. The BES mission is to develop understanding and to stimulate innovative thinking needed to fortify the Department's missions.

The program has two distinct interrelated parts: research and facilities operations and development. In the pursuit of forefront research results, BES designs, builds and operates certain large, complex advanced scientific facilities such as neutron sources and synchrotron radiation sources. These facilities not only provide BES with unique instruments, but these instruments are also made available to all qualified users, even those not supported by BES. Thus, the facilities actually leverage a great deal more research from the national effort.

Research to broaden the technology base supporting either specific energy options or generic energy research is extremely important. Equally important, however, is the need for continuing basic research, unconstrained by preconceived notions of which technologies will be important several decades from now, so that new, as yet unidentified, options may emerge. A comprehensive program of basic energy-related research and fundamental knowledge-seeking research in topics of interest to DOE is essential.

The BES program conducts basic research that will most likely help the Nation's long-term energy goals. BES implements a broad strategy for conducting basic research and contributes strongly towards national energy goals and to national goals of maintaining and enhancing scientific leadership, technological innovation, and economic strength.

The following pages describe the program of the Department of Energy's Office of Basic Energy Sciences. The BES subprograms and facilities are discussed, along with an abbreviated budget summary and an outline of plans for the future. Any reports referenced are available from the National Technical Information Service, U.S. Department of Commerce, Springfield, Virginia 22161.

Overview

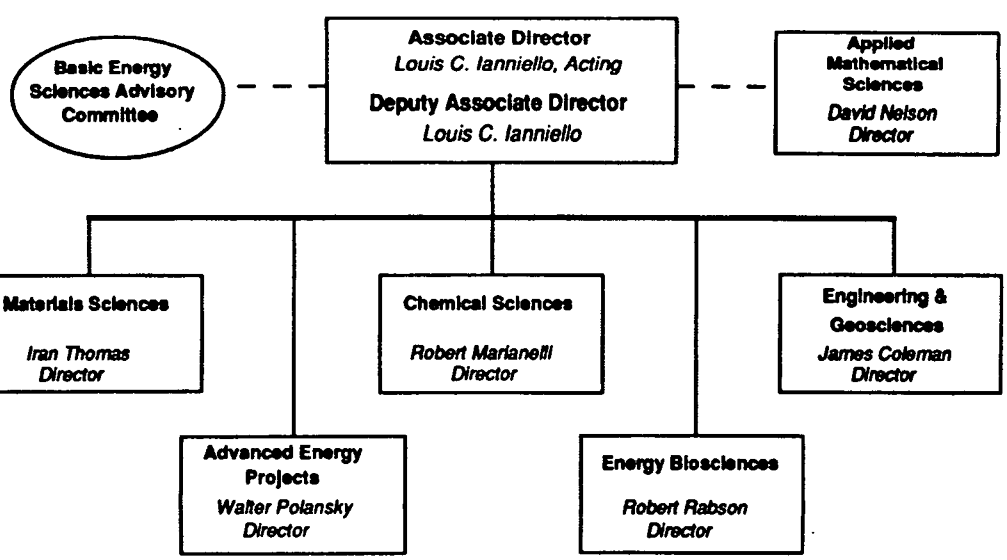
Basic research requires long-term commitments of resources and people with the promise only of long-term success and long-term return on investment. Thus, the private sector, dominated by concerns for high and rapid return on investment and other short-term considerations, is playing a lesser role in support of basic research than it did during the past few decades. As a result, support of long-range basic research has become the special responsibility of the Federal Government.

Within the Department of Energy (DOE), the mission of the Office of Energy Research (ER) is to support advanced research aimed at gaining insights into the behavior of nature. The Office of Basic Energy Sciences (BES) is responsible for long-range basic energy-related research. The BES goal is to provide the scientific underpinning needed to develop energy options for the future.

The Office of Basic Energy Sciences plans and administers DOE's programs of basic energy research. BES is organized primarily along scientific discipline lines as shown in Figure 1. This structure helps the basic research community align themselves with the BES support units. Nevertheless, topics of interest to DOE often cross these divisional boundaries. Examples of such topics include catalysis and surface science involving both Materials Sciences and Chemical Sciences subprograms, photosynthesis and photochemistry involving both Chemical Sciences and Energy Biosciences subprograms, and mechanical fracture involving both Materials Sciences and Engineering and Geosciences subprograms.

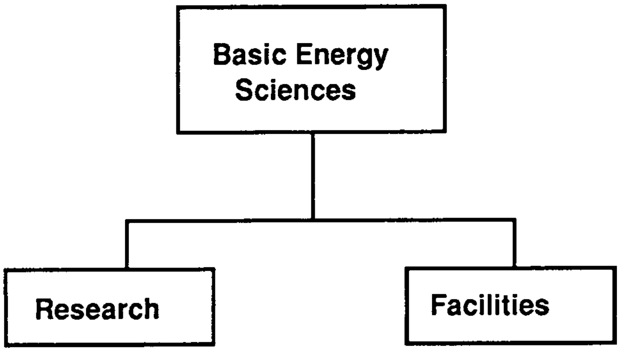
Figure 1.

Office of Basic Energy Sciences



BES also has an important responsibility to design, build and operate complex scientific facilities. This responsibility flows from the nature of the program, to carry out forefront research, and from the talent that exists uniquely at the DOE laboratories. The BES program, in a functional sense, thus consists of two parts, research and facilities, as depicted in Figure 2.

Figure 2.



Characteristics of the BES program are: long-term generic basic research underpinning the Nation's technology base and fortifying foundations for the Department's missions; support of research at universities and at the national laboratories which support the educational objectives of the Department; and design, construction and operation of complex scientific facilities for the national user community. Throughout the Nation, BES supports about 1,400 research projects, each selected because of its scientific and technical merit and its relevance to the Department's research objectives.

The knowledge gained through BES-sponsored research becomes an integral part of the body of information needed for the Nation's technology base.

DOE's laboratories are national assets that play an essential role in U.S. science and technology. Expert scientific and engineering staffs exist at the laboratories; complex scientific facilities are operated by the laboratories and are accessible to academic and industrial researchers; and inter-disciplinary projects are undertaken at the laboratories on topics of national importance. Much of the BES budget that goes to the national laboratories is to operate complex facilities, support research dependent on them, and provide services uniquely available at the laboratories. The nature of the facilities and the character of BES programs have made BES a major contributor in the evolving national goal of enhancing our economic competitiveness through more rapid exploitation of scientific results for technology applications.

Many areas of modern science depend on large and costly facilities to develop information not otherwise attainable. The unique facilities in the BES program are made available for use by the entire scientific community. The operation of major scientific facilities requires a large commitment of BES funds. These facilities include the National Synchrotron Light Source at Brookhaven National Laboratory; the Stanford Synchrotron Radiation Laboratory; the Combustion Research Facility at Sandia-Livermore; the High Flux Isotope Reactor at Oak Ridge National Laboratory; the High Flux Beam Reactor at Brookhaven; the Intense Pulsed Neutron Source at Argonne National Laboratory; the Manuel Lujan, Jr. Neutron Scattering Center, LANSCE, at Los Alamos National Laboratory; and high-voltage and atomic resolution microscopes.

Most of the scientists involved in BES research programs are located at universities and national laboratories. In addition, access to qualified scientists not directly supported by BES is provided at the major user facilities. Thus, while about 25% of BES funding directly supports university-based research, indirect support for university research also is significant. Besides universities and national laboratories, BES maintains ties with industry. Industrial scientists serve on the Basic Energy Sciences Advisory Committee; experts from industry participate in the review of research proposals and use the specialized facilities sponsored by BES; industrial scientists participate in program advisory committees at the national laboratories; and industry representatives are invited to attend BES conferences and workshops. Through these and other mechanisms, research results become available to industry in a timely fashion.

The BES program also participates in the Governmentwide-mandated Small Business Innovation Research Program which was initiated in Fiscal Year 1983. A number of BES projects are being supported at research-oriented, small business firms. The level of this effort was 1.25% of the BES operating expenses in Fiscal Year 1990 -- i.e., about $5,400,000.

Interagency information exchanges, committee interactions, and workshops provide liaison between BES and other research groups. For example, DOE offices and laboratories and such Federal agencies as the National Science Foundation, the Nuclear Regulatory Commission, the U.S. Geological Survey, and the Department of Agriculture have working groups and committees that routinely exchange information and coordinate program activities in areas of common interest such as chemistry, geophysics, materials, combustion, and plant sciences research. Coordinating committees discuss individual proposals and compare work being done by the various agencies to avoid undesirable overlap and duplication of effort. Outreach workshops and working groups bring together investigators in related areas to share information and discuss related problems in their work. The results of these interactions normally are published in the open literature to make them available to the scientific community worldwide.

Special Topic

Basic Energy Sciences Support
for Research Relevant to More
Efficient Energy Systems

Introduction

The Basic Energy Sciences program is very broad in scope and difficult to summarize in a single document. Each issue of the Basic Energy Sciences Summary Report, therefore, attempts to focus on only one area of research to provide the reader with information on the BES approach, accomplishments, and activity centered around one theme. This year, the subject selected is ***"More Efficient Energy Systems".***

In the following examples, the reader can begin to appreciate the concept of basic research which leads to more efficient energy utilization. In some cases, totally unexpected results lead to advances; in others, there is steady progress towards an established objective. Long lead times are required in most cases to actually see the fruits of basic research in specific applications. Basic research involves the replenishment of the storeroom of knowledge. Without that knowledge and understanding of the world around us, the drive for advances in technology would disappear. These examples are only a few of the many BES research activities which contribute to more efficient energy systems.

Intermetallic Alloys for High-Temperature Energy Systems

Ordered intermetallic compounds[1] based on aluminides and silicides constitute a unique class of metallic materials that have promising physical and mechanical properties for structural applications at elevated temperatures for energy generation, conversion, and conservation. Major interest has focused on the aluminides of nickel, iron, and titanium due to their resistance to oxidation, low densities, and high melting points. The properties which have made these ordered alloys interesting are high-yield strength and high modulus, low density, high work-hardening rate, and low steady-state creep rate. They show greater strength (deform more slowly) at elevated temperatures and show less oxidation than conventional alloys. However, until very recently, these materials were thought to be extremely brittle so that they were only used in structural applications as second phase particles to strengthen an alloy. Indeed, their brittleness had prevented their being fabricated into useful forms.

Intermetallic compounds have been known since the early 1900's, but they did not attract much attention until the 1950's, when work at the GE Research Laboratory and the University of Birmingham (England) indicated that they had interesting mechanical properties.[2] Extensive

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[1] C. T. Liu, J. O. Stiegler, and F. H. Froes, "Ordered Intermetallics," in Metals Handbook, 10 ed. Vol. 2, Properties and Selection: Nonferrous Alloys and Special Purpose Materials. ASM Handbook Publ.; 1990. pp. 913-42.

[2] Robert W. Cahn, "Load-Bearing Ordered Intermetallic Compounds - A Historical View," MRS Bull. 15 [5]: 18; 1991.

studies of ordered intermetallics were carried out until the late 1960's, when interest waned due to the severe embrittlement problems. The most highly ordered intermetallics were found to be so brittle that they could not be simply fabricated into structural components, and fabricated materials were found to have a low fracture toughness.

In the 1970's, C. T. Liu and his collaborators at Oak Ridge National Laboratory (ORNL) showed that macro-additions of iron to the intermetallic compounds Co_3V and Ni_3V increased their ductility by more than 40% due to changing the crystal structure from hexagonal to cubic. In 1979, Aoki and Izumi[3] showed that micro-additions of boron dramatically increased the ductility of polycrystalline Ni_3Al. By the early 1980's, the ORNL group, led by Liu, showed that the boron was segregated at the grain boundaries and suppressed brittle intergranular fracture. However, the mechanism by which boron suppressed intergranular fracture was not understood until very recently. Likewise, the source of the brittleness in Fe_3Al and FeAl was not understood until recently.

In the quest for the explanation of the brittle behavior of Ni_3Al, Fe_3Al and FeAl, the ORNL group and other national laboratories and university research groups supported by the DOE's Basic Energy Sciences have played key roles. The BES program has supported both experimental and theoretical studies which have provided a fundamental understanding of the causes of low ductility and brittle fracture in these aluminides. For instance, a significant advance has been made in mechanistic understanding of yield strength and brittle fracture of ordered transition metal aluminides on the basis of quantum mechanical total-energy calculations, atomistic simulation modeling, and anisotropic elasticity theory of dislocations and cracks.[4]

Ni_3Al has excellent strength, is oxidation resistant at elevated temperatures, and is the most important strengthening component in nickel-based superalloys. Single crystal Ni_3Al is ductile at ambient temperatures, while the purest polycrystalline Ni_3Al fails by grain-boundary fracture. The ORNL results not only showed that small boron additions (~0.1 wt%) eliminated the brittleness of polycrystalline Ni_3Al but converted the material into a highly malleable form with a ductility as high as 50% at room temperature. Most importantly, ductility was sufficient enough to permit the fabrication of components of these alloys by standard metallurgical procedures. The improved ductility was found to be realized only in alloy compositions containing less than 25 at% aluminum. Segregation of boron was observed to be less strong in aluminum-rich alloys. Carbon, which is similar to boron, does not have a comparable effect; and iron, chromium, manganese, or beryllium which enter substitutionally must be added in much larger additions to effect a small improvement in ductility.

Ni_3Al with boron and improved alloys based on it have much improved high-temperature strengths compared to established materials such as Hastelloy X and 316 stainless steel. These improved Ni_3Al-based alloys have potential uses in gas, water, and steam turbines for energy generation and turbochargers, pistons and valves for improved automotive performance. ORNL, through a DOE technology program, has led the way in developing large-scale processing of advanced Ni_3Al alloys using standard metallurgical procedures. This work has yielded a new class of alloy materials for demanding structural applications.

The beneficial effect of boron has been explained by two mechanisms. One mechanism proposes that B, which segregates at the grain boundaries, increases the cohesive energy of the grain boundaries to the extent that stress concentrations at the grain boundaries are relieved by slip and not by fracture. The second mechanism suggests that B enhances dislocation generation and eases transmission of slip across grain boundaries. The effect of boron on ductility is unique.

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[3] K. Aoki and O. Izumi, J. Japan Inst. Met. 43: 1190; 1979.

[4] M. H. Yoo and C. L. Fu, "Fundamental Aspects of Deformation and Fracture in High-Temperature Ordered Intermetallics," Iron and Steel Institute of Japan (ISIJ) International, Special Issue on Advanced High Temperature Intermetallics (in press).

Recently, Lee, Subramanian, Robertson and Birnbaum[5] at the Materials Research Laboratory, University of Illinois, in another BES sponsored project, obtained strong experimental evidence supporting the mechanism by which B increases the cohesive energy of grain boundaries so that stress concentrations are relieved by slip in grains adjacent to the grain boundary. By using the chemical analysis techniques available in a scanning transmission electron microscope, they were able to rule out the existence of a wide second phase at grain boundaries and enhanced Ni concentration in the neighborhood of grain boundaries. They were able to observe the interaction between matrix dislocations and grain boundaries directly by deforming samples in-situ in a transmission electron microscope, thus allowing them to observe differences between alloys with and without boron. They observed that the grain interiors were ductile and dislocations piled up at grain boundaries. The dislocations that had entered the boundary did not dissociate into grain boundary dislocations or move along the boundaries as expected if boron eased the slip transmission process. Instead, they found that in alloys containing B the stress concentration at grain boundaries was relieved by slip transmission into adjacent grains, while in B-free specimens the stress was relieved by nucleation and propagation of intergranular cracks.

Fe_3Al and FeAl, while not having the exceptional strength of Ni_3Al, have corrosion resistance to many agents. The U.S. Navy attempted to develop Fe_3Al and ternary alloys based on it in the 1950's, but was forced to give up the effort due to its brittleness at ambient temperature (see footnote[2]). C. T. Liu and his collaborators at ORNL took up the effort again very recently in a study of compositions between FeAl and Fe_3Al, with Mo, Cr, TiB_2, and other additions. Under BES support, they have succeeded in identifying the embrittling factor in these intermetallic alloys. They found that the alloys are intrinsically quite ductile and that poor ductility results from embrittlement by a reaction with air.[6] The Al in the intermetallics at surfaces is thought to react with water vapor to form aluminum oxide (Al_2O_3) and atomic hydrogen. The atomic hydrogen migrates into the intermetallics and causes brittle cleavage fracture at ambient temperatures.

The experimental results were supported by a theoretical study carried out by C. L. Fu and G. S. Painter at ORNL.[7] Their quantum mechanical calculations of the bonding characteristics, the bond and cleavage strength between iron and aluminum layers, and the surface energies with and without interstitially absorbed H showed that FeAl is intrinsically resistant to cleavage fracture in terms of the high theoretical cleavage strength. Further, they found that the effect of hydrogen on the bonding between Fe and Al layers is dramatic. Hydrogen locally dilates the lattice, and there is a concentration-dependent decrease in Fe-Al cleavage strength. These results suggested that the underlying mechanism of H-embrittlement in aluminides is a depletion of bonding charge on the Fe site resulting from an Fe to H charge transfer.

Alloys involving FeAl and Fe_3Al may find applications in such energy areas as coal combustion. The BES supported program at ORNL has identified the cause for embrittlement of these alloys. Based on this knowledge, it has been clear that attainment of ductility requires the control of surface composition and properties, and a program for metallurgical processing of FeAl and Fe_3Al alloys has been designed. With DOE technology support, Liu and his group at ORNL have pushed ahead with the development of these materials. In 1990, C. G. McKamey, V. K. Sikka and C. T. Liu's development of ductile iron aluminides was recognized with a R&D 100 award by R&D Magazine. Industry has expressed an interest in both the iron and nickel aluminides and several licenses for commercialization of processes have been granted for alloys of the two types of intermetallic materials.

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[5] T. C. Lee, R. Subramanian, I. M. Robertson and H. K. Birnbaum, Scr. Metall. 26: 1265-70; 1991.

[6] C. T. Liu, E. H. Lee, and C. G. McKamey, Scr. Metall. 23: 875; 1989.

[7] C. L. Fu and G. S. Painter, "First Principles Investigation of Hydrogen Embrittlement of FeAl," J. Mater. Res. 6 [4]: 719-23; 1991.

High-Temperature Superconductors

When high-temperature ceramic superconductors burst upon the world scene with their discovery by Bednorz and Müller late in 1986, and subsequent reports of new ceramic materials with superconductivity occurring at temperatures as high as 125 K (-148 °C), many applications were immediately anticipated for their use. Cables that would conduct large currents with no resistive losses and large-scale superconducting coils for magnetic energy storage (SMES) systems were envisioned to achieve unprecedented energy efficiency. Ceramic superconductors also offered significant improvements in the form of superconducting motors, generators, and transformers; superconducting magnets in advanced energy-conversion devices such as tokamaks; high-field magnets for magnetohydrodynamic and magnetically levitated transportation systems; etc. Immediate use of these materials, however, was frustrated by problems with their brittleness, difficulties in fabrication, their reactivity with the environment, low current-carrying capacity, and the loss of superconductivity.

Although major scientific and technical problems with these new superconducting materials greatly slowed the realization of any significant application, an understanding of these materials and the superconducting phenomena occurring in them has been slowly gained during the past five years of intensive research. Interest has been sustained in the belief that these materials will have potential for many diverse applications. The National Commission on Superconductivity recommended a major national effort to develop and use wire made with high-temperature superconductors, and the importance of developing this technology was repeated by the recent 1990 Annual Report of the National Action Plan on Superconductivity.

DOE has had a long-standing interest in superconductivity because of its use in high energy physics and fusion. Traditionally, DOE has had the largest Federal program in superconductivity. Since high-temperature superconductivity has a significant prospective application in electric power systems, a broad range of research was undertaken in 1987 and subsequent years. This research was directed toward the fundamental science of high-temperature superconductivity and the use of high-temperature superconductors in a variety of energy-related technologies.

Principal responsibility for fundamental research programs is located in the Office of Basic Energy Sciences, while the largest portion of the technology program is supported through the Office of Energy Storage and Distribution (OESD). BES supports major programs at Ames Laboratory, Argonne National Laboratory (ANL) and Oak Ridge National Laboratory (ORNL), plus smaller programs at four other national laboratories and about 15 universities. The technology programs are carried out at the national laboratories and in companies from the communications, power, manufacturing, and superconductor industries. The BES-supported program at ANL is an example of research which is concerned with fundamental questions of high-temperature superconductivity yet is closely related to an OESD program to develop ceramic superconductors for cables and storage coils. With efforts to develop cables and storage coils, it has become abundantly clear that a firm understanding of the underlying physics and materials science of these materials is required in order to make significant progress.

Virtually all energy applications require the superconducting material to carry large electrical currents. In the superconducting state, electrons travel through a material without being deflected (scattered) by atoms in the material. However, at defects and grain boundaries in the superconductor and at regions where magnetic field lines penetrate through the material, the crystal structure that enables superconductivity to occur is interrupted and scattering of the superconducting electrons takes place giving rise to resistance losses. The preparation of suitable practical conductors has posed numerous problems related to anisotropy effects, grain boundary imperfection, control of magnetic flux lattice in the presence of magnetic fields, and control of second-phase impurities.

The overriding issue here is the control of microstructure by the control of defects and impurities. Although this issue is also of considerable importance for conventional superconductors, it has become critical for the high-temperature superconductors, where numerous aspects that were not previously known have become apparent. In the past year, significant progress has been made to identify many of the mechanisms which limit the current-carrying capacity of these materials, and in preparing materials with improved properties. The principal problem seems to lie with the current flow across grain boundaries.

Many of the applications of superconductors which require large current-carrying capacity arise from their use in producing large magnetic fields, in which case the superconductors are permeated by a lattice of magnetic field lines. Due to an interaction between the electric current and the magnetic field, these field lines tend to move through the material, causing a dissipation which is equivalent to an electrical resistance and leads to a rapid reduction in the current. The presence of non-superconducting defects and impurities can pin the magnetic field lines to the crystalline lattice, which inhibits their motion and removes the current dissipation. Recent work has made significant progress in defining the defects which can produce such an effect and in preparing materials which carry much higher currents.

Defects effective in magnetic flux pinning consist of regions which are non-superconducting. These defects can be either intrinsic (arising from the nature of the material itself) or extrinsic (added to the materials from the outside). The structures of many high-temperature superconductors consist of one or more two-dimensional layers of Cu-O separated from one another by regions of non-superconducting material. Careful measurements of the current in a single crystal of $YBa_2Cu_3O_{7-\delta}$ have shown that these intermediate layers themselves can provide pinning for the case when the magnetic field lies in the Cu-O plane. This phenomenon, whereby even the perfect material provides some of its own flux pinning, is unknown in conventional superconductors. It is well known that even single crystals of high-temperature superconductors break up into crystallographic domains which are oriented at an angle relative to one another, and are separated by "twin boundaries". Because chemical composition changes at these boundaries, the boundaries are not superconducting, and measurements have now demonstrated that they may provide pinning sites.

Extrinsic defects may be added to the material in a variety of ways, one of the most interesting being by radiation damage. It has now been demonstrated that bombarding these materials with various radiations, including neutrons, protons, and various ions, can produce very small defects which alter the microstructure in such a way that the current-carrying capabilities are enhanced without destroying the superconducting properties. On a large scale, control of the synthesis of the material can result in very small, highly dispersed precipitates of non-superconducting material which pin the flux. These results demonstrate that the microstructure may be manipulated to produce the best material in a variety of ways.

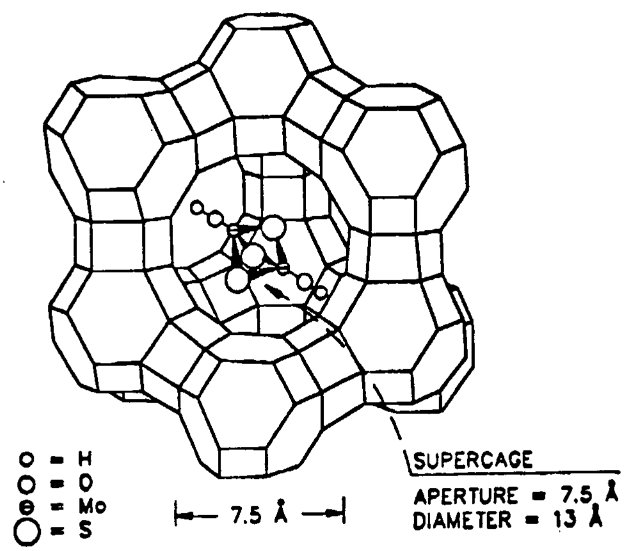
In polycrystalline materials, the current carrying properties of the high-temperature superconductors are primarily dominated by the grain boundaries between different crystallites. As with the twin boundaries discussed above, the grain boundaries are non-superconducting. However, the grain boundaries may actually interfere with the transport of current between crystallites, unless the crystallites are accurately aligned with one another. This has been greatly clarified by recent high-resolution electron microscopy on $YBa_2Cu_3O_{7-\delta}$ which has shown that misaligned grains result in numerous areas along the boundary, "dislocation cores," formed to accommodate the alignment mismatch, with the number of cores depending on the degree of mismatch. These dislocation cores appear to be Cu-rich and non-superconducting. At sufficiently low density, they may act as pinning centers in the manner described above, but when there are so many of them that they overlap one another, they effectively form a barrier which inhibits the transport of current. The most effective way found to deal with this problem is to process the bulk material so that the grains are aligned. One approach has been to subject polycrystalline material to zone refined, partial melting procedures. This has been demonstrated at several institutions, but Argonne has done extensive work to optimize the thermal parameters and has also shown that the addition of small amounts of Ag can enhance the final purity of the material. In this way, textured products have been formed which possess a uniform grain-aligned microstructure over their 50 mm length. While this process is currently too slow to be commercially useful, it has demonstrated that uniform high-current materials can be produced.

Although substantial work remains before one obtains mass-produced, high-quality bulk conductors, the recent progress has been remarkable. There are grounds for optimism concerning the future of high current-carrying superconducting ceramics.

Catalysts for Methane Conversion

Workers at the Argonne National Laboratory (ANL) are seeking to exploit a series of discoveries, made in the course of BES-sponsored materials research, that could pave the way for more efficient and effective utilization of natural gas in the production of fuels and industrial chemicals. Methane, the principal ingredient in all natural gas deposits, can be converted to more useful, higher molecular weight hydrocarbons in the laboratory, but only with great difficulty. The principal approach to methane conversion that is under study worldwide involves the use of catalysts composed of selected metal oxides, mixed metal oxides, or doped metal oxides. Conversion schemes based on this approach require temperatures in excess of 600°C and the presence of oxygen in some form to sustain the reaction. The high-temperature constraint reduces overall process efficiency and makes it necessary to use exotic construction materials, while the oxygen promotes side reactions that cause an undesirable oxidation of methane and hydrocarbon products to CO and CO_2.

Figure 3.



Sketch of a large pore molecular sieve with a built-in, catalytically active inclusion compound (in this case a $Mo_2S_x(OH)_y$ cluster). Molecular sieve catalysts like this one are being developed for novel hydrocarbon transformation reactions, including direct methane coupling to produce fuels and industrial chemicals.

The technique under investigation at ANL utilizes a family of microporous materials called molecular sieves (Figure 3) that contain built-in metal ions with novel catalytic properties. A number of highly reactive metal ion centers have been incorporated into synthetic molecular sieves, some substituted at framework metal atom positions and others synthesized in the form of clusters within the pores and cages of the sieve structure. Several different constituent compounds in this latter configuration have exhibited the capacity to attack the C-H bonds of methane catalytically at temperatures as low as 400°C and without the need for oxygen. The successful development of an industrial process based on this type of molecular sieve catalyst could have profound implications for the petroleum and petrochemical industries.

The goal of the ANL research project is to synthesize a catalyst that both activates the C-H bonds of methane and controls the size of the product molecules. The C-H bond activation is accomplished when the methane molecules come in contact with the special metal ion centers incorporated in the molecular sieve, while the size selectivity is achieved because of the microporous nature of the sieve structure. Current emphasis is on catalyst systems capable of converting methane to low molecular weight hydrocarbons, such as ethane and ethylene at temperatures as low as 400°C. These products could subsequently be converted to liquid fuels and chemical feedstocks by conventional industrial synthesis methods. If this project is successful, the process of patenting the inventive aspects will be completed and one or more industrial partners will be sought for further collaborative development work leading to pilot scale testing and demonstration.

Geochemistry in Oil Exploration

A key element in the development of more efficient energy systems is full exploitation of the Nation's energy resources. The National Energy Strategy emphasizes the efficient and environmentally acceptable use of oil and gas resources for the near-term. The United States has been producing oil and gas since the mid-1800's, making it the most experienced nation in the world regarding oil and gas production. The extensive oil exploration activities of the past, however, make it unlikely that large new fields comparable to those in the Middle East will be found in the U.S. This limitation places a great deal of emphasis on developing technology for efficient exploration and utilization of hydrocarbon resources that we have on hand and those likely to be discovered. Efficient utilization, in turn, requires a fundamental understanding of origin, migration, and accumulation, leading to better ways of finding new reserves and of producing, by conventional means, the remaining two-thirds of oil-in-place.

Because of the enormous cost necessary to discover, develop, and produce oil and gas from sedimentary basins, oil companies attempt to improve their drilling successes by learning as much as possible about the structure of subsurface rock formations and their oil-bearing potential prior to drilling. In combination with methods to evaluate the thermal history of sedimentary basins, geochemical data can be used to determine the timing of hydrocarbon generation and the generative capacity of any source rocks present. Geochemists at Lawrence Livermore National Laboratory (LLNL) have developed improved chemical kinetic models of oil generation, cracking to gas, and expulsion from the source rock. These models are now widely used in the oil industry.

Oil is derived primarily from the lipid fraction of phytoplankton and zooplankton, the microscopic organisms floating in the upper layer of lakes and oceans. The remains of these organisms, together with those of bacteria that process the debris after it falls to the bottom, are eventually buried in the oxygen-free sediments accumulating in an ocean or lake. This organic matter, consisting of solid cellular debris and dissolved compounds, coalesces through chemical and biochemical reactions occurring in the upper portion of the sediment column into a highly insoluble substance of complex molecular structure called kerogen.

Continued burial through accumulation of additional sedimentary layers subjects the kerogen and the enclosing sediment, now rock, to higher temperatures and pressures. Under these conditions, portions of the kerogen structure break off to form free hydrocarbons. Initially, the compounds include a significant component of higher molecular weight hydrocarbons that are only slightly modified from their original biochemical precursors. Further heating of the kerogen and these initial products to higher temperatures produces smaller and smaller hydrocarbons and a more carbon-rich kerogen. The ultimate products of this molecular cracking process, if allowed to continue to completion in a closed system, are methane and graphite. Some of the larger molecular weight hydrocarbons may leak out of the source rock into shallower formations before they can be cracked to gas. If sufficient quantities of these larger hydrocarbons migrate from the source rock, they may eventually be trapped by an impermeable seal, and an oil reservoir begins to form.

Our understanding of the oil generation process has been acquired through a combination of detailed geological and geochemical studies of oil and gas bearing sedimentary basins and laboratory experiments intended to duplicate natural hydrocarbon generation in the laboratory. The conversion of kerogen to oil and gas is a chemical reaction, the rate of which depends on temperature. Reactions that require millions of years in nature at about 100°C take only hours or days in the laboratory when the experiments are accelerated at temperatures of 250-350°C. Retorting of oil shales at high temperatures to obtain commercial quantities of oil is simply a variation of the geochemists' laboratory experiments carried out on a grander scale.

The most sophisticated petroleum generation models now in use were developed by a team of geoscientists at LLNL. These models grew out of the Oil Shale Project funded through the DOE-Morgantown Project Office. The LLNL team, led by Alan Burnham and including Robert Braun and Jerry Sweeney, realized in the early 1980's that the chemical kinetic models that they had developed for oil shale pyrolysis had advantages over those then in use for oil exploration. The team measured rates of oil generation from a variety of source rocks and adapted their oil shale pyrolysis codes to models of hydrocarbon generation in sedimentary basins. They wrote the computer code KINETICS to analyze data from laboratory experiments and to derive the parameters necessary for predicting the timing and quantity of oil generation. KINETICS is designed to be user-friendly for non-experts and to run on personal computers.

Congress has mandated that the national laboratories should actively seek technology transfer arrangements with U.S. companies to enable them to benefit from Government-sponsored research. With DOE's agreement, the University of California obtained a copywrite on KINETICS and licensed it for commercial distribution to two companies in 1987 and 1988. The software has since been acquired by 16 oil companies, three universities, and two Government laboratories. These sales, which greatly increased the project's visibility within industry, led to the formation in 1988 of an Industrial Sponsorship Program. For their successful technology-transfer efforts in petroleum geochemistry, the LLNL group received a Federal Laboratory Consortium 1990 Award for Excellence in Technology Transfer.

With encouragement from the industrial sponsors, the geochemists adapted another code, PYROL, also written for the oil-shale retorting project, for use in oil exploration. Because PYROL is too complicated and not user-friendly, the group developed another code, PMOD, that is easier to use and offers greater flexibility. Both codes are used to calculate the volumes of oil and gas generated at all stages of burial and the efficiency of petroleum expulsion under various organic carbon contents and burial rates. Users can specify these variables based on independent assessment, or they can assume different values to obtain a range of possible outcomes. Further refinements in the code will deal with the role of pressure and chemical type in oil cracking.

This project is an excellent example of the sometimes very close relationship between basic and applied research. Laboratory experiments provide fundamental data that is incorporated into a code describing the reactions in the chemical system under investigation.

The codes are then adapted to simulate conditions in nature. Industrial code users provide feedback to the research team based on their experiences in applying the code to oil exploration. The researchers then improve their code based on further experimentation and modeling. In addition to BES support, the LLNL group also has funding from DOE's technology divisions and industry sponsors. The BES funding continues to support the basic laboratory experimentation underlying the code development.

More Efficient Imaging of the Earth's Crust

Until fairly recently, the three-dimensional nature of the earth's interior was revealed for only the shallowest portions of the earth's crust by the processes of natural erosion and by man-made excavations and drillholes. The need for infor-mation about the third dimension has grown enormously as man has tried to understand and control his immediate environment, including his search for natural resources. Since the development of practical seismic reflection tools for oil exploration in the 1930's, the need for direct access, via drill holes, for subsurface information has been progressively and substantially replaced by geophysical imaging techniques geotomography. These techniques are based on measuring the velocity, attenuation, phase shift, and scattering of seismic-acoustic and electromagnetic (EM) waves as they pass through the earth between a set of energy source points and another set of receiver points. Sources and receivers may be at the surface, underground, or in any combination of surface and underground locations.

EM techniques are primarily sensitive to spatial variations in the amount and temperature of conductive fluids in rock voids and to the concentration of certain types of conductive minerals. In reservoir or fluid flow problems, for example, EM can be used to infer the type of fluid present (oil vs. brine) and to indicate zones of different saturation, porosity or fracture density. Because of the higher resolving power of seismic techniques, seismic tomography tends to be better for resolving lithologic discontinuities, but seismic tomograms also reveal information about fluids present (viscosity and saturation) and something about rock properties (porosity/fracturing).

In contrast to images produced by medical tomography, the first geotomographic images obtained between boreholes gave rather crude and imprecise parameterizations of geologic conditions. A part of the difficulty with early geotomograms arose because of the lack of good sources and receivers. Also, the algebraic reconstruction techniques assumed waves propagating along straight raypaths. Processing algorithms had to be developed for more complicated geologic conditions, more powerful subsurface sources had to be developed for adequate signal levels between wells, and better rock physics information had to be obtained before geotomography could be properly applied to real-earth problems.

Electromagnetic Imaging

The Geosciences program in BES is one of the most active research programs in electromagnetic geotomography. The initial impetus came from a need to develop more accurate and deeper-probing surface methods for mapping the three-dimensional electrical conductivity distributions around young volcanic complexes such as Long Valley Caldera, California, and the Valles Caldera, New Mexico, which were sites of scientific drilling under the U.S. Continental Scientific Drilling Program (CSDP). Out of these studies came improved instrumentation, data collection methodologies, and data interpretation algorithms for both the magnetotelluric (MT), a natural field method, and controlled-source field methods.

In controlled-source research, Morrison, et al., at Lawrence Berkeley Laboratory (LBL), have looked at the viability of utilizing ultra-large sources to achieve better signal strengths. This work showed that while controlled-source methods have inherently better resolution than MT, and will have an important role in shallow imaging, improvements in technology make MT a better means for imaging at depths over 1 km.

Because MT relies solely on natural broadband, ultralow-frequency, electromagnetic energy supplied through the dynamic interaction between the solar wind and the earth's main magnetic field, signal strength cannot be controlled. The observed magnetic and electric fields consist of a spatially coherent signal and a sometimes larger incoherent noise due to cultural and natural sources; signal and noise exhibit complex fluctuations. Moreover, near-surface conductivity heterogeneities (geologic noise) cause severe distortions in the local electric field components of the data.

Researchers at LBL have developed linear filtering algorithms to remove the effects of near-surface geologic noise, and researchers at Oregon State University have developed improved algorithms for recognizing and deleting noisy data segments in each frequency band. In complementary studies, researchers at Los Alamos National Laboratory (LANL) and the University of Washington have been developing faster and more robust methods for inverting large MT data sets. As a result of this work, MT practitioners are far better able to obtain high quality data and useful subsurface conductivity images than in the past.

For a number of practical reservoir and contaminant plume problems, it is important to detect and monitor the changes in subsurface resistivity with a high level of resolution by means of borehole sources and receivers. Researchers at LLNL have been developing a technique, called electric resistivity tomography or ERT, in which the earth is imaged using dc current electrode sources in boreholes. This technique has already been applied to leak detection at a surface pond.

Seismic Tomography

An early accomplishment of the Geosciences program in this area was the development of the Sandia Downhole Seismic Source, a resonant swept-frequency vertical dipole source that produces mainly vertically polarized shear waves that propagate in the horizontal direction. As an important new tool for crosswell seismic tomography, it was first deployed for scientific projects in 1981. Since then, the tool has been used on a number of applied technology projects, and has been substantially improved with the result that the current tool has a larger moment, higher frequency capability and lighter weight. It has been turned over to Bolt Technologies, Inc., for commercial applications.

The ability to turn the raw seismic data into useful images of the earth between boreholes (a process referred to as inversion) has been a continuing challenge because of the hetergeneous nature of the earth. James Berryman, LLNL, has developed a novel computational approach for traveltime tomography reconstructions that makes no a priori assumptions about the raypath taken by the first arriving seismic signal between any source and receiver location. Using feasibility constraints based on Fermat's principle that states the path must be the one of least traveltime, he models both the raypaths and the spatial distribution of velocities.

Whether for crosshole or conventional surface seismic exploration, it is necessary that one be able to compute synthetic seismograms. These are representations of the wavefields at any point due to sources in an arbitrarily complex earth. In this regard, computationally efficient and accurate ray-tracing algorithms have been developed at the Center for Wave Phenomena (Colorado School of Mines) which are well-suited to problems of high-resolution imaging of topologically complex geologic structures such as salt diapirs and recumbent folds. Dave Hale and Jack Cohen have developed software that converts any two-dimensional model into a mesh of triangular elements. This type of mesh has a number of appealing features important to the problem of ray tracing, such as great flexibility in handling velocity variations within or between triangles and the capability for extending the process to three dimensions.

Emulsion Phase Contractor: Efficiency in Separations

Methods to separate two dissimilar chemical species are used extensively in both analytical and production processes, and the efficiency of a separation process is often a major factor in determining the cost of a manufactured product. The extraction of one liquid from another requires methods which optimize contact between the two liquid phases. The normal means of achieving significant contact uses pumps and impellers to drive the two phases together in an appropriate vessel and relies on the resulting turbulence for adequate mixing of the liquids.

An entirely original approach to this problem was developed at Oak Ridge National Laboratory, patented, and recently licensed for commercial development. In this new approach, water containing the chemicals to be separated flows through a nozzle between two electrodes. Upon application of a pulsed electric field to the electrodes, the water is dispersed into extremely small droplets, thus increasing the surface area of contact between the dispersed and liquid phases. Tests with laboratory-scale versions of this so-called Emulsion Phase Contactor prove it to be at least a factor of 10 more effective than the industry standard, while requiring a factor of 100 less energy for its operation. Licenses have been granted to Analytical BioChemistry Laboratories of Columbia, Missouri, to exploit the method in analytical equipment and to the National Tank Company of Tulsa, Oklahoma, to develop large-scale extraction equipment for application in processing systems for the metals and petroleum industries. The concept evolved from basic research supported by the Division of Chemical Sciences and was subsequently developed under funding from the Division of Advanced Energy Products, both in the Office of Basic Energy Sciences.

TRUEX and SREX: Efficiency for Waste Isolation

Other research in separation science has had significant indirect impact on energy efficiency.

The work of Dr. E. Phillip Horwitz, a research chemist at Argonne National Laboratory, has resulted in new, vastly more efficient approaches to the processing of spent fuels from nuclear reactors. An organic molecule known as CMPO, designed and synthesized by Dr. Horwitz and his group, exhibits the highest affinity for transuranic elements, or TRU, of any known organic compound. It is now commercially available in industrial quantities from Atochem North America, Philadelphia, Pennsylvania. TRUEX, an industrial scale process to remove TRU from nuclear wastes based on the CMPO molecule, is now in the engineering design phase at the DOE Hanford site in Washington State. Because of the greater affinity for actinides exhibited by the CMPO molecule, the volume of radioactive waste which must be immobilized and placed in deep isolation can be reduced by more than a factor of 100 below that projected on the basis of previous extraction technology. The increased efficiency of the TRUEX process will significantly reduce the cost of waste remediation for both civilian and nuclear wastes. Dr. Horwitz received the Department of Energy Distinguished Associate Award in 1990 for the research leading to the development of the TRUEX process.

More recently, the Argonne group adapted a commercially available crown ether for use in a process, known as SREX, to remove strontium from nuclear waste. This advance will further reduce the volume of material requiring deep isolation.

Combustion

The goal of high-efficiency utilization of fuels in combustion processes is often at odds with another important goal: minimized production of pollutants. The conditions required for high efficiency, such as high burning temperature, typically elevate the levels of species such as nitrogen oxides (NOx) in exhausts above what they are for lower-efficiency combustion processes. Only by understanding the detailed reactions through which NOx is produced and destroyed can scientists and engineers design engines and other combustors that preserve efficiency while minimizing pollution. The Division of Chemical Sciences in BES supports fundamental research in the chemical kinetics of combustion processes and emphasizes understanding the reactions that lead to the production and destruction of NOx and soot, two of the major unwanted by-products of combustion. An illustrative example of how BES-supported work is leading to practical advances is the development of a process for removing NOx from combustion exhausts. A BES researcher investigating elementary chemical reactions important to the combustion chemistry of nitrogen realized that his work had implications for NOx removal. He redirected his research to study a process that has become known as RAPRENOx, for the RAPid REduction of NOx. Applied research supported by what is now DOE's Conservation and Renewable Energy Branch followed and showed the practical promise of the process. The scientist who conceived RAPRENOx, Robert A. Perry, became so interested in the practical implications of his work that he formed TECHNOR, a company that is now testing its application to a variety of devices, including commercial diesel engines.

Catalysis

The presence of a catalyst allows a process to be carried out at a lower temperature than would be possible in its absence, thereby increasing the energy efficiency of the process. The industrial importance of catalytic processes is reflected in the fact that fully 17% of the GNP depends on catalysis. Increased understanding of catalytic processes gained from BES-supported research has reduced the heat required to convert naturally occurring alkanes into more useful fuels and chemicals. The simplest and most abundant alkane, methane, is an exceptionally unreactive molecule, but is a readily available natural resource. In order to make this abundant resource useful for chemical processes it must be converted to a more reactive form. Because of its innate stability, heat must be supplied to achieve practical conversion rates. Five years ago the temperature required was in excess of 1000K. Recent research at both Texas A&M and Lawrence Berkeley Laboratory has produced composite surfaces that enable the conversion process to occur at temperatures below 850K.

That the unexpected is often the most useful product of basic research is illustrated by related work at Yale University. While studying a particular catalytic reaction, the investigator added mercury as a standard test for precipitation of the catalyst under study. A totally unexpected, but desirable, reaction was observed. It was subsequently determined that the unexpected reaction was itself catalyzed by mercury. This work led to the development of the MERCAT process, a new approach to the conversion of alkanes to more valuable chemicals and fuels. The MERCAT process is conducted at temperatures only slightly above ambient and will lead to significant energy savings.

Photochemical Conversions

Research in solar photochemical energy conversion seeks more direct routes to the use of the vast untapped energy available in the form of sunlight to produce electricity and to convert raw materials, such as water and carbon dioxide, into high-energy fuels. Significant advances of the last decades in understanding natural photosynthesis and in controlling electron transfer processes are providing insight into design of artificial photosynthetic systems. This work recently produced the first synthetic molecules which duplicate in large measure the properties of natural photosynthetic systems. The BES program supports fundamental research on a myriad of credible pathways to efficient photochemical conversion ranging from molecular organic and organometallic photoredox systems to heterogeneous photocatalytic arrays and semiconductor/liquid junctions. By the next few decades, several of these may reach the developmental stages and begin to impact future global energy production.

Work supported by Basic Energy Sciences in the Chemical Technology Division in Oak Ridge National Laboratory demonstrated the first simultaneous photoevolution of molecular hydrogen and oxygen in a synthetic mixture comprised of isolated natural chloroplasts, ferredoxin, and hydrogenase. Methods were developed to deposit platinum directly on chloroplasts, thus forming a composite material to which electrical contact could be made. It was subsequently shown that a two-component system comprised of these platinized chloroplasts could perform the same water splitting reaction. These results are significant because they demonstrate an unambiguous thermodynamically uphill reaction in which hydrogen is the energy-rich photoproduct rather than the carbon dioxide fixation compounds of normal photosynthesis. Information produced by this work may lead to efficient methods to use photochemistry for renewable production of fuels and chemicals. Current research at Oak Ridge National Laboratory is focused on understanding the photobiocatalytic and molecular bioelectronic properties of the new composite material.

Membrane Science

Synthetic membrane processes are substantially more efficient than many other separation processes because the energy needed to induce phase changes is not required. For example, the membrane process used for generation of potable water from sea water, known as reverse osmosis, requires about 30% less energy than conventional distillation. A major impediment to further improvement in the efficiency of membrane process is membrane fouling. In the case of reverse osmosis, membrane efficacy deteriorates with time because protein molecules adhere to the membrane surface and reduce the effective pore size. Fundamental research to determine the nature of the interaction between membrane materials and protein molecules is supported by the Division of Chemical Sciences at Rensselaer Polytechnic Institute. Increased understanding of the origin of this interaction may lead to definition of the chemical properties of the membrane surface which will minimize protein fouling. Significant further energy savings could be achieved.

Nanophase Materials

The assembly of matter by the condensation of gas-condensed atomic clusters is probably as old as the universe itself, since this is thought to be the way in which matter condensed after the "big bang," yet the successful application of this approach to form ultrafine-grained materials is a very recent development. A major part of this development occurred in a BES-supported program at Argonne National Laboratory with the work of Richard Siegel and his collaborators.[8] Investigations of the formation of ultrafine particles or atomic clusters by condensation from a gas was undertaken by a few laboratories in Japan and Europe in the 1960's and 1970's, and the formation of ultrafine-grained materials was suggested by Professor H. Gleiter in 1981. The Argonne effort has entailed the synthesis of metal and ceramic powders, the compaction and densification of the powders into solid bodies, and investigations of material properties. In a short period of 5 years, the Argonne work has been carried to the point where a small commercial firm has been "spun off" to carry out commercial development and production of ultrafine-grained materials.[9]

Nanophase materials are ultrafine-grained materials in which the grains are in the size range of a few nanometers (nm) up to 100 nm, where one nanometer is 1 billionth of a meter. Nanophase materials may consist of grains of more than one type (i.e., phase) of compound or crystal structure, hence these materials are generally referred to as "nanophase". Since the grains are submicroscopic in size, many of the atoms in a grain lie at or near the surface of a grain. A nanophase material with a 5 nm average grain size will have from 30 to 50% of its atoms associated with grain boundaries. Consequently, the properties of nanophase materials are expected to be governed largely by the properties of the grain boundaries and confined grain dimensions.

Although the grains in nanophase material are so small and the atoms in a grain lie close to grain boundaries, the interior of the grains tend to show a high degree of crystalline perfection. Grains also tend to be equiaxed in shape. Examination of ultrafine-grained palladium (Pd) and rutile (TiO_2) at ANL showed that grain boundaries resemble grain boundaries in coarser grained materials in that they tend to be flat, with some faceting and to have short-range ordered structure resembling that of the bulk material. These materials, surprisingly, showed very little grain growth when heated. For example, rutile did not show appreciable grain growth until heated above 800 °C.

Nanophase materials differ from conventional materials in having some properties that are different and often considerably improved. The ANL group showed that TiO_2 could be sintered under ambient pressure at temperatures 400 to 600 °C lower than that for conventional material, while maintaining grain size and shape. Material densified under pressure to full density had a greater microhardness than conventional material. Nanophase rutile could be plastically deformed to such a degree that is was possible to form it to near-net shape. Nanophase palladium showed greatly increased strength, with a yield stress of 249 MPa (megaPascals) as compared to a yield stress of 52 MPa for conventional material.

Some unique advantages of the assembly of nanophase materials from gas-condensed clusters, and the nanophase processing method based on this, are as follows:

(1) The ultrafine sizes of the atom clusters and their surface cleanliness allow conventional restrictions of phase equilibria and kinetics to be overcome during material synthesis and processing by the combination of short diffusion distances, high driving forces, and uncontaminated surfaces and interfaces.

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[8] R. W. Siegel, "Nanophase Materials Assembled from Atomic Clusters," MRS Bull. 15 [10]: 60-67; 1990.

[9] Press release, Argonne National Laboratory.

(2) The large fraction of atoms residing in the grain boundaries and interfaces of these materials allow the interface atomic arrangements to constitute significant volume fractions of materials and, thus, novel materials properties may result.

(3) The reduced size scale and large surface-to-volume ratios of the individual nanophase grains can be predetermined and can alter and enhance a variety of physical and chemical properties.

(4) A wide range of materials can be produced in this manner including metals and alloys, intermetallic compounds, oxide and nonoxide ceramics, and semiconductors. It is also apparent that nanophases can be formed with crystalline, quasicrystalline, or amorphous structures.

The introduction of advanced materials obtained under novel synthesis and processing conditions can lead to increased efficiency in a wide range of applications. The National Energy Strategy notes that an enhanced research and development effort is expected to accelerate the development of new, efficient fuel-diverse automobile technologies, and includes the development of automotive gas turbines, high-temperature ceramic materials, and friction-reducing technologies as key areas requiring development. Replacing traditional materials with advanced material systems offers many advantages. For example, higher operating temperatures in engines and the use of lighter weight, stronger materials lead to improved fuel efficiency. Such needs can only be met by advanced materials including ceramics, intermetallics and composites.

According to a recent survey by the U.S. Bureau of Mines, advanced structural materials will require higher strength-to-density ratios, greater strength and toughness, and superior thermal properties as compared to "traditional" materials. Due to their high-temperature mechanical properties and relative light-weight, ceramics and ceramic composites are among the most promising materials for many applications. Poor fracture toughness and fatigue/creep properties, lack of processing reliability, and high cost are major impediments for the commercial application of these materials. Solution of these problems will require advanced techniques for processing ceramic materials, as well as the development of new synthesis techniques for materials with enhanced physical properties.

The synthesis of nanometer-size atom clusters of metals and ceramics by means of atom-cluster condensation in a gas, followed by the <u>in situ</u> consolidation of clusters under high-vacuum conditions, has resulted in the past few years in a new class of ultrafine-grained interface materials. These nanophase materials, with average grain sizes that presently range from 100 nm down to about 5 nm, offer considerably improved properties for advanced technologies. The gas-condensation method for the synthesis of nanophase materials appears to have great flexibility and control for engineering new forms of bulk nanostructured materials.

Current research has indicated that considerable enhancement of desirable properties is obtained by virtue of the small grain size and large grain boundary area. These properties will enhance the ability to manufacture components and will reduce energy requirements and production costs. Ultrafine-grained ceramics with increased toughness and strain rate sensitivity can be formed rapidly to near net shape and machined without breaking. Increased diffusion rates, resulting in increased densification rates, make possible greatly reduced sintering temperatures for the formation of bulk materials. Increased diffusion rates also make possible the incorporation of other components (dopants) into the material to control properties or to form special electronic materials.

The rapidly developing opportunities for synthesizing nanophase materials via the assembly of atom clusters are just beginning to make an impact on materials science and technology. However, based upon the limited but growing knowledge that has already been accumulated, the future appears to hold great promise for these new materials. The ability to produce via cluster assembly metals with increased yield strength and fully dense ultrafine-grained nanophase ceramics that are rapidly formable can have a significant technological impact in a wide variety of applications. Much is still not understood about this new class of materials in which properties are largely controlled by the grain boundaries, but it appears clear from the outset that they offer much in the way of improved materials, improved ease of manufacture and reduced energy cost.

Eliminating Weld Failure in Energy Generating Systems

Boiler tube weld failures are the primary cause of central power station boiler-forced outages.[10] Forced outages are often long and expensive due to needed repairs and lost power production. Failure of one tube supplying steam to a 500 MW unit, assuming 72 hours to repair, can cost a utility as much as $700,000 in fuel transfer costs alone. If improved welds made coal-fired plants available for service 1% more of the time, the power industry would save $1.2 billion over a 5-year period (see footnote[1] on page 5). Welded joints that are reproducible and reliable with long service lives are crucial to reducing the number of failures and thereby to improving the overall performance of power plants.

To a large extent, the integrity and performance of welded structures depend on the microstructure-property relationships within the weld. Unfortunately, many of the basic principles relating weld performance and properties to welding processes and to the weld microstructure are not well understood. The needed welding science is a complex field that must encompass a wide spectrum of fundamental physical and applied sciences.

DOE's Basic Energy Sciences Welding Science Program is the only major, long-term basic welding research program in the United States. The program endeavors to provide the necessary thrust and leadership to advance welding science and technology. The BES Welding Science Program, through Oak Ridge National Laboratory (ORNL) and several collaboratory university projects, addresses a wide range of topics related to the basic understanding of the evolution and stability of weld microstructures, the properties of weldments (i.e., the unit formed by welding together two pieces of metal), heat and fluid flow, mass transfer, welding processes, and welding consumables.

Hot-cracking that occurs during welding is a significant problem that is encountered in welding a wide variety of alloys. Such cracking reduces the weldability of materials and leads to rejection of welded components. ORNL is investigating the fundamental causes of hot-cracking. Solidification behavior and the evolution of the weld microstructure are being examined by controlled experiments using highly characterized stainless steel single crystals. The effect of alloying impurities is also being studied by experiments with controlled additions of tramp elements. The single crystal studies have already provided some basic insights into the development of weld grain structure and solidification substructures. The principles that the program has established regarding microstructural development and its relationship to hot-cracking have been applied to improve the weldability of iridium alloys that are used as structural containment material for radioactive fuel in thermoelectric generators for outer planetary missions.

Thermal history and fluid flow in welds determine the weld pool shape, solidification behavior, and structure of welds. This information is critically needed before predictions of weld microstructure or properties can be made, yet it is difficult to obtain experimentally. Weld process modeling is a powerful tool that provides a means for obtaining this information. ORNL is developing a mathematical model that can provide quantitative relationships between key process parameters, resultant heat flow and fluid flow in the weld pool, and the structure and properties of the weld

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[10] Joining Dissimilar Metals Conference Proceedings, AWS and EPRI (August 1982).

produced. These relationships can be used to predict weld pool geometry and, thus, to insure the reliability of welded joints.

The performance of welds in service at high temperatures depends on the stability of the microstructure of the weldment. Microstructural instability can lead to degradation in weld properties such as overall embrittlement of welded structures. Austenitic stainless steels are used extensively in power plants for high-temperature service. ORNL has shown that austenitic stainless steel welds are subject to embrittlement over a wide range of temperatures. Causes for this embrittlement have been identified that should lead to avoiding degradation of properties through alloy and process modification. One potential solution that is being investigated at ORNL is the use of high energy density processes such as laser and electron beam welding. ORNL has demonstrated that these processes can prevent formation of undesirable and unstable phases such as ferrite in austenitic stainless steel welds through rapid solidification effects.

Thick-section pressure vessel steels are commonly used as components of power plants, and welding is an integral part of the fabrication of such components. Conventional welding processes such as shielded metal arc and submerged arc welding are commonly used techniques, but they are time consuming and expensive. As an alternative to these processes, the feasibility of electron beam welding of thick-section steel was examined. Such a process offers several advantages with regard to cost, speed, and the elimination of filler metals. Thick section (4 to 6 in.) welds have been shown to be produced successfully with excellent properties.

The BES Welding Science Program also supports research at Pennsylvania State University, the Colorado School of Mines, and, until recently, a successful now-completed program at the Massachusetts Institute of Technology (MIT). These university projects collaborate closely with the work at ORNL.

Researchers at Pennsylvania State University are concerned with understanding alloy element vaporization from weld pools since significant loss of alloying elements during welding can affect microstructure-property relationships and, thus, the integrity of welds. They are developing a comprehensive theoretical model to predict from first principles the rate of alloying element loss and resulting changes in the weld metal composition.

The research at MIT is also theoretical and is aimed at developing a comprehensive mathematical representation of heat and fluid flow during arc welding. The investigation addresses a critical issue of two-way coupling between heat source (welding arc) and the weld pool.

Finally, the work at the Colorado School of Mines addresses the important issue of the role of compositional and microstructural gradients on weld metal properties and behavior. By the nature of the welding operation and associated thermal cycle to which the material is subjected, a significant gradient in both microstructure and composition exists in a weldment. This is the case in the fusion zone, or weld metal, and in the adjacent heat-affected zone. These gradients can adversely affect the weldment structure and its properties and, thus, the integrity of the weldment. The program at the Colorado School of Mines is characterizing the extent of these gradients and their influence on the performance of weldments.

In the area of welding control, a collaborative project involving MIT and the Idaho National Engineering Laboratory has focused on developing the foundation for fully automated gas metal arc welding. To accomplish that, the research has led to the utilization in a control system of visual information about the state of the weldpool. Current work has implemented advanced techniques, such as neural nets and fuzzy logic, for a prototype welding control system which is capable of learning. Some of the results are sufficiently advanced to have attracted direct support by the U.S. Navy.

BES-sponsored welding research has led to a greater understanding of the relationship between welding process, microstructure, and properties. This type of fundamental understanding can lead to improved production and performance of welded structures in power plants and other energy generating systems. However, further effort is required before a complete understanding of welding phenomena is achieved.

Subprograms

Basic Energy Sciences research is conducted through its five divisions and the Scientific Computing Staff.

Materials Sciences

It is well known that materials problems and limitations often restrict the performance of current energy systems and the development of future ones. The goal of Materials Sciences is to increase the basic scientific understanding of how matter in the condensed state behaves, what its properties are under different conditions, how they relate to structure, and what phenomena are involved in and govern behavior. This understanding is essential to the development of future energy technologies. Some practical objectives to which Materials Sciences research ultimately contribute include:

- *Developing new or substitute materials;*
- *Tailoring materials to meet design performance requirements;*
- *Predicting materials problems and service life;*
- *Improving the ability to anticipate and resolve unforeseen materials problems in advanced energy systems; and*
- *Improving the theoretical and experimental capability to analyze and measure the basic structure and properties of materials, and predict the behavior of potentially promising new materials.*

Examples of research accomplishments this past year include:

1. ***Record Organic Superconductor Transition Temperature***

   An organic superconductor, based on a copper containing charge-transfer salt, having the highest superconducting transition temperature yet obtained, 12.5K at 0.3 kbar pressure, was synthesized at Argonne National Laboratory (ANL). The slight applied pressure was found to be necessary to suppress a semiconducting transition at 42K, thereby giving rise to the superconductivity. The previous record transition temperature for an organic superconductor of 11.6K was also discovered by the same group at ANL.

2. ***A New Mechanism for Surface Diffusion***

   A new mechanism for atomic diffusion on surfaces was discovered. In this new mechanism, diffusion occurs by a replacement process between the surface absorbed atom (adatom) and a substrate surface atom. The adatom "burrows" into the substrate surface while a substrate atom "pops up" onto the surface at another site. This mechanism is known as a concerted-displacement process. From a scientific perspective, the discovery of this new mechanism implies that metal atom surface diffusion cannot always be viewed as a single atom hopping along the surface. The discovery also has technological implications in that processes such as the manufacture of alloys and corrosion prevention often involve the incorporation of atoms into a surface.

3. ***Birth of Molecular Tribology***

The first direct measurements of both the static and dynamic properties of ultrathin liquid films between two surfaces sliding past each other have been made. These measurements mark the birth of molecular tribology, the study of friction and lubrication at the atomic scale. The measurements of the properties of such lubricating films, only a few molecular layers thick, trapped between surfaces, are crucial for determining the adhesion, friction, lubrication, and wear characteristics of engineered surfaces in mechanical systems. The measurements on the films showed that the properties are profoundly different from those of the bulk. Changes were observed in both static properties such as density and molecular orientation, and dynamic properties, e.g., viscosity, shear strength and molecular relaxation times. Magnitude difference between films and bulk properties range up to 10 orders of magnitude.

4. ***Interfacial Force Microscope with Atomic Scale Resolution***

A new electrostatic force feedback sensor was developed at Sandia National Laboratories which has extended the sensitivity of the atomic force microscope, a device used to investigate forces between two surfaces at an atomic level with atomic resolution. In this new force feedback sensor design, the stiffness of the force sensor is controlled through an electrostatic balancing force that is, itself, controlled by an electronic feedback loop. In this approach, the interfacial force is measured through the voltage of the feedback circuit. This corrects problems with instabilities that occurred in previous microscopes when the sensor tip approached the test surface. The new stability permits measurements from large separations down to within an atomic diameter of the test surface.

5. ***Double Rotation Nuclear Magnetic Resonance***

A new approach to the nuclear magnetic resonance (NMR) technique led to the invention and development of the double rotation method at the Lawrence Berkeley Laboratory. The results permit the NMR investigation of solid materials with resolutions approaching those obtained for liquid samples. Line broadening has long inhibited the application of NMR to solid samples; the constrained motion of the atoms in solids produce non-symmetric interactions. The so-called magic angle spinning developed in the 1950's partially solved the problem of line broadening in solids for atoms with spherical nuclei. However, many nuclei of technological importance are not spherical. The new technique solves this problem by spinning the sample around two mathematically defined axes. Two separate approaches have been taken; one involves the simultaneous spinning of the sample about the two axes, the second involves a rapid sequential spinning about first one then the second axis. Both are found to work. The technique has already attracted widespread attention and interest.

6. ***New Hydrogen-Defect Center in Gallium Arsenide***

A new defect center was discovered in the compound semiconductor gallium arsenide which is formed by the binding of a hydrogen atom impurity to an arsenic atom. Hydrogen ion bombardment is presently used to produce electrical and optical isolation in gallium arsenide integrated circuits, but the degrading role of this defect center was not understood. The arsenic-hydrogen defect center was observed by infrared vibrational spectroscopy following implantation of hydrogen ions at cryogenic temperatures. The hydrogen bonding was demonstrated through a shift in the absorption frequency upon isotopic substitution of the deuterium isotope of hydrogen, whereas the role of arsenic was deduced from observations of a similar arsenic-hydrogen center in indium arsenide. The arsenic-hydrogen center becomes unstable at temperatures above 250K, giving way to a previously known gallium-hydrogen center.

7. ***Self-Segregation In Multicomponent Technological Ceramics***

Scientists at the Oak Ridge National Laboratory have shown that when a totally random mixture of two different granular materials have sufficiently different sizes, shapes, or other physical properties, segregation of the components can occur during certain types of processing of technological materials. If a random mixture is poured into another container, the nonlinear dynamics of the granular flow leads to the almost total segregation of the two constituents. The final distribution of the granules in the new container shows a concentration of the more mobile constituents at the bottom and the periphery of the pile with the less mobile species near the center and top. The flow of granular material composed of more than one type of constituent is common in material preparation, especially in technological ceramics. Typically, various materials are mixed in one container and then poured into another for sintering. Self-segregation under such conditions can significantly affect the final form of the treated material. In fact, such self-segregation, experimentally observed, led to the modeling effort and subsequent explanation of the phenomenon.

8. ***Chemistry Provides Clues to Avoiding Stress-Corrosion-Cracking of PWR Cladding***

Recent results strongly suggest that carbon can greatly reduce the stress-corrosion cracking in pressurized water reactor (PWR) cladding through the formation of very stable carbon-centered zirconium cluster iodides. The experiments resulted from predictions made three years ago at the Ames Laboratory. PWR fuel elements from the Chalk River nuclear research complex in Canada are composed of a graphite-uranium dioxide dispersion where the graphite was believed to act as a lubricant. The experiments showed that mixtures of cladding materials such as zirconium with graphite and iodine reacted at 320 °C, a representative inner wall temperature of a PWR fuel system in operation to form the carbon-centered zirconium iodides as predicted. These cluster carbides were also detected in a burned fuel rod. Experiments are underway to extend the observations to working systems which are typically too radioactive to examine easily. This work should lead to a new understanding of the role of graphite dispersions in reducing stress-corrosion cracking of the cladding in PWR fuel rods and, ultimately, to new rod designs.

9. ***High Purity Ceramic Oxide Crystal Growth Using a Containerless Plasma Process***

A process for the growth of high purity ceramic oxide crystals at temperatures greater than 2000 K has been developed. This process uses an inductively coupled plasma, which has the advantage of providing sufficient heat to melt materials with high melting temperatures and is essentially containerless, ensuring a high purity crystal. Video imaging and computer feedback control provide real-time control of the process. Key to the control of the process is the understanding of the interrelationships among the various process variables; the most important of the process parameters is the position of the crystal within the plasma and the powder feed rate. The use of real-time video monitoring coupled with computer controlled crystal motion has allowed precise positioning of the crystal such that a shape preserving crystal growth can be maintained.

10. ***Embrittlement of Intermetallics; Significance of Alloy Additions***

Results from the University of Illinois Materials Research Laboratory have shown that the addition of boron to the technologically important intermetallic, nickel aluminide dramatically improves the crack-resistant properties of the material. The reaction of the intermetallic, with and without boron, to stresses is extensive plastic grain flow; dislocations pile up against the boundaries forming local stress concentrations. It was shown in this work that when boron is segregated to grain boundaries, the grain boundary is strengthened sufficiently to allow the stress concentration to be relieved by initiation of dislocation generation in the adjacent grain. In the absence of boron, the response of the grain boundary to the stress concentration is crack initiation, which then propagates along the grain boundary leading to premature intergranular fracture.

11. *Superplastic Behavior in Nanocrystalline Titanium Dioxide*

For the first time, a fully densified nanophase ceramic, titanium dioxide, has been synthesized and several of its mechanical properties measured. Methods have been developed at the University of Illinois Materials Research Laboratory to synthesize dense ceramic materials with grain sizes of 10-15 nm using nanophase processing. The technique permits the synthesis of nanophase ceramics that can be fully densified while still retaining their ultra-small grain size. Stress-strain rate measurements have been made. Preliminary analysis of the grain size dependence and stress exponents suggests that in such ultra-fine grained materials as these nanophase ceramics, diffusional creep may be limited by the efficiency of sources and sinks of point defects in the grain boundaries rather than the mobility of defects, as previously assumed. This work also demonstrates, for the first time, that nanophase ceramics can be superplastically deformed to close to the final shape in a single step and that the unique microstructure of nanophase materials provides a means to investigate deformation mechanisms.

12. *Direct Observation and Control of a Precipitate Shape Transformation*

The first direct observation of a controlled and reversible, solid-state precipitate shape transformation was made using the high penetration and hot stage of a 1.5 million volt high voltage electron microscope (HVEM). Small germanium precipitates in an aluminum matrix were found to undergo a reversible transformation from a strongly faceted to a rounded shape during temperature cycling. The observations demonstrated, for the first time, that it is possible to change the shape of a given type of precipitate from an extremely anisotropic shape -- an octahedron, bounded by eight triangular faces -- to a completely isotropic shape, a sphere. Furthermore, by rapid cooling, different shapes can be stabilized. The strength of lightweight, high-performance alloys such as those used in aerospace and automobile applications depends on the shape and coherence of inclusions and precipitates to the matrix.

13. *Basis of Toughness Enhancement Shown for Silicon Carbide Whisker/ Alumina Ceramic Composites*

Mechanical interlocks between surface serrations on silicon carbide whiskers and an amorphous silicon dioxide film on the surface of the whiskers were shown to be the microstructural basis of toughness in silicon carbide whisker-alumina composites. Detailed observation of the interface with high resolution electron microscopy (HREM) showed that the interface affects the toughness of a composite through the mechanical interlocks. The depth of the serrations influences the amount of silicon dioxide at the interface. Fabrication of the composite yielded interfaces with reduced silicon dioxide film thicknesses when compared to the film present on the whiskers prior to fabrication. The amount of retained interfacial silicon oxide depended on the processing conditions as well as on the local topography of the interface; the more deeply serrated interfaces retained more silicon oxide. Whisker surface morphology, as well as the initial amount of amorphous silicon dioxide on SiC whiskers, are important variables in determining the toughness of the ceramic composite.

14. *New Method for Transmission Electron Microscopy; Z-Contrast Imaging of Atomic Structures*

A new high-resolution electron microscopy technique was developed at Oak Ridge National Laboratory. Images produced by this technique depend on both the atomic positions, as in conventional transmission electron microscopy (TEM), and the atomic number of the imaged atom -- hence the name Z-Contrast. The method, which uses the wide-angle scattered illumination generated by the scanned incident electron beam, has a demonstrated resolution of .22 nm. A new model is now under construction; this model is expected to have a resolution of .14 nm, a resolution better than any yet achieved in electron microscopy. This development has earned a R&D 100 award.

15. ***Corrosion Kinetics of Ceramics in Electrolytes Explained***

A new quantitative model that successfully predicts corrosion rates of ceramics in electrolyte solutions was developed at the Pacific Northwest Laboratory. The model, based on electrical surface charge phenomena, models the change in the concentration of hydrogen ions at the ceramic surface as the surface charge varies due to changes in electrolyte concentration and composition. Experimental results for alkali silicates and alkali aluminosilicates in alkali chloride solutions are in good agreement with the model's predictions and confirm that it is the local surface concentration of hydrogen ions and not the bulk solution value that most strongly affects corrosion rates of such ceramic materials. The discovery of the relative importance of the local surface chemistry rather than bulk solution chemistry in driving aqueous corrosion processes in ceramics is significant for the development of strategies to minimize the corrosion of ceramic components in aqueous solutions.

16. ***Hardening and Improved Wear of Aluminum by Oxygen-Ion Implantation***

Implantation of oxygen-ions into aluminum was shown to produce near-surface hardness comparable to that of high-strength steel, to reduce sliding friction by more than 60% and to suppress catastrophic galling wear. Microindentation of one-half micrometer implanted layers revealed flow stresses several times greater than previously achieved for any aluminum alloy. This strength resulted from the unique implantation-produced microstructure. The aluminum matrix contained 20 volume percent of nanometer-size aluminum oxide precipitates, and these strongly impeded dislocation motion. The large improvements in friction and wear were observed in unlubricated sliding tests where the implanted aluminum disc moved against a steel pin.

Superconductivity

Following the discovery in late 1986 of "high-temperature" superconductivity (the observation of superconductivity above the boiling point of liquid nitrogen), BES laboratory and university scientists undertook a variety of research activities aimed at understanding the phenomena observed. Some results of superconductivity-related research are reported here.

1. ***High Sensitivity, High Temperature Superconductivity SQUID Magnetometer Developed***

A thin film Superconducting QUantum Interference Device (SQUID) magnetometer with unprecedented sensitivity, made entirely from high-temperature superconductors, was fabricated and tested at the Lawrence Berkeley Laboratory (LBL). The magnetometer consists of two magnetically coupled components: a dc SQUID fabricated from a thallium-calcium-barium-copper oxide superconductor and a flux transformer fabricated from a yttrium-barium-copper oxide superconductor. The photolithographically fabricated flux transformers work at temperatures up to 84K and can now be prepared reproducibly. Coupled with the new SQUIDs, the result is a magnetometer for use at liquid nitrogen temperatures with a magnetic field amplification of over 80 and a sensitivity to 0.3 picotesla. Improvements in sensitivity, noise reduction and fabrication reproducibility are continuing. The magnetometer is already suitable for some applications in geophysics and nondestructive testing.

2. ***Identification of the Superconducting Energy Gap in High Temperature Superconductors***

The energy gap between the band of electronic states responsible for superconductivity and the normal electronic states was identified in several high-temperature ceramic superconductors for the first time. An important question with regard to high-temperature superconductors is the location of the energy band which is occupied by the paired electrons responsible for the superconducting current. This band is known to lie sightly above the highest normal electron energy level, called the Fermi edge, and to be separated from the normal levels by an energy gap. In a collaborative effort among the Ames Laboratory, Los Alamos National Laboratory, and Argonne National Laboratory, the Fermi edge was clearly seen experimentally for the first time, and a superconducting gap was identified. The superconducting gap in one ceramic superconducting compound was measured to be 24 millielectron volts. These results provide essential experimental knowledge which is needed for the establishment of theoretical models.

3. ***Large Improvements in Current Carrying Capacity of High Temperature Superconductors by Irradiation***

Large improvements in the electrical current carrying capacity of high-temperature ceramic superconductors were achieved when the samples were irradiated with either ions or neutrons. Electron microscopy investigations showed a cellular microstructure developed as a consequence of moderate irradiation doses of neon or krypton ions. The same microstructure was found to occur after neutron irradiation. A comparison of neutron and ion irradiation results suggested that the cellular microstructure was produced most effectively by high energy recoils which helped to explain why different types of irradiations produce different variations in superconducting properties. This work showed that the critical current was optimized at low neutron doses. By selection of irradiation conditions that optimize the microstructure for the current carrying capabilities, while simultaneously maintaining other important material properties, high temperature superconductors can be used in energy applications where high currents are required and high magnetic fields are present.

4. ***Metallic Precursors Yield Manufacturable Microcomposite Superconductors***

Oxidation of melt-spun precursor metallic ribbons of bismuth, lead, strontium, calcium, copper, and silver was shown to yield a microcomposite of a high-temperature superconductor material with a high critical current density. The process appears capable of yielding a variety of long wires and ribbons. The microcomposite consisted of a mixture of the ceramic superconductor and silver metal. The composite material has good formability and can be mechanically pressed or rolled. The superconducting transition temperature is about 105 K. The critical current density, which is a measure of the superconductor to carry current without losing its superconductivity, is only a factor of 5 below the highest value quoted for continuous wire processing. Multiple stacks of ribbons, long wires, and ribbons can be fabricated by cladding and rolling; also, the superconducting wire can be joined to normal metal wires. Superconducting wires produced with this method exhibit good environmental stability, showing no degradation of electrical transport properties even after immersion in water for 30 days.

5. ***Electronic Structure of the Yttrium-Barium-Copper Oxide Ceramic Superconductor***

The electronic structure of the ceramic superconductor yttrium-barium-copper oxide was calculated using the quantum mechanical method known as the Orthogonalized Linear Combination of Atomic Orbitals (OLCAO) method. This calculation yields representations of the electronic charge density around the atoms in the crystal structure, the electronic energy bands (dispersion relations), electron density of states, and optical properties. A further calculation was performed to aid the interpretation of positron annihilation experiments and yielded an estimate of the overlap of electron and positron densities which are related to the positron annihilation rate. Based on a comparison of theoretical and experimental results, it was concluded that the change in the positron annihilation rate below the superconducting transition temperature is critically related to the transfer of charge from the planar oxygen atoms to the apical oxygen atoms in the crystal lattice.

Materials Sciences is coordinated within the Federal Government in part through the Interagency Committee on Materials (COMAT) and within the DOE in part through the Energy Materials Coordinating Committee (EMaCC). The panel reports of the Division of Materials Sciences' Council on Materials Science (a body with representatives from academia, industry, and agency laboratories) workshops and Research Assistance Task Forces help to focus attention on critical issues. One recent panel study covered the subject Fundamental Issues in Hydrogen-Defect Interactions. The Division of Materials Sciences also sponsored three workshops on topics related to the Division's research programs. These were: Radiation Effects on Materials in High-Radiation Environments; Highly Conducting Ceramics; and Welding Science.

More detailed information on the activities of the Materials Sciences subprogram can be obtained from I. L. Thomas, Director, Division of Materials Sciences, Office of Basic Energy Sciences, Department of Energy, Washington, D.C. 20585, (301) 353-3427. A detailed summary of current projects is published annually. The most recent (January 1991) is entitled "Materials Sciences Program, Fiscal Year 1990" (DOE/ER-0483P).

Chemical Sciences

The Chemical Sciences subprogram sponsors experimental and theoretical research on liquids, gases, plasmas, and solids. The focus is on their chemical properties and the interactions of their component molecules, atoms, ions, and electrons. The subprogram objective is to expand, through support of basic research, our knowledge in the various areas of chemistry; the long-term goal is to contribute to new or improved processes for developing and using domestic energy resources. At a budget level of $155,600,000 in Fiscal Year 1991, this subprogram is a major source of Federal support for basic chemical research in the United States. Disciplinary areas covered include physical, organic, and inorganic chemistry; chemical physics; atomic physics; photochemistry; radiation chemistry; thermodynamics; thermophysics; separations science; and analytical chemistry.

Chemical phenomena and processes apt to be important to energy technologies are considered in formulating the program. Included is research that impacts fields such as photovoltaics, i.e., the conversion of solar energy to electricity; production of fuels and chemicals from coal; catalysis; nuclear waste separation and management; conversion of biomass, i.e., wood or leafy materials into liquid fuels using enzymes or microorganisms; separation of metals from low-grade mineral resources; combustion; and detection, measurement, and remediation of harmful by-products of energy processes.

Research in some areas, such as chemical catalysis to learn why some molecules may uniquely promote specific chemical reactions, may be quickly exploited by industrial process designers. Research in other areas, such as photochemistry -- light-induced chemical reactions -- to produce hydrogen from water decomposition, may not find practical application for a number of years even though scientific strides are being made. Still other research areas, such as the study of the interactions of atoms and electrons with plasmas, may produce knowledge important in the development of new energy technologies.

Equally important is the fundamental research into chemical processes and phenomena that are not immediately identified with a particular energy technology. A typical example of such an effort is the study of molecules, atoms, or ions which have been impacted by laser beams, have energy levels above normal and, thus, may show unusual chemical behavior.

Examples of research accomplishments this past year include:

1. ***Yttrium-90 for Cancer Treatment: A New Process***

   A new process for the removal of strontium-90 (^{90}Sr) from nuclear waste has been adapted to the preparation of yttrium-90 (^{90}Y) in high yield and with purity required for region-specific cancer treatment. The separation is accomplished by chromatographic adaptation of the SREX and TRUEX processes developed for extraction of Sr and transuranic elements, respectively, from nuclear waste. The source material consists of the fission product ^{90}Sr separated from nuclear waste. The ^{90}Y isotope accumulates as a result of beta decay of ^{90}Sr. Sr is, therefore, always present in the source material but, for medical applications, its concentration must be reduced to a level below 100 parts per billion (ppb). This level is achieved with three chromatographic stages. The first two employ columns based on the SREX process to remove Sr. The third stage uses a column based on the TRUEX process to sequester the remaining ^{90}Y. The ^{90}Y is recovered by treating the stationary phase from the TRUEX column with water. Because of the specificity of the TRUEX process, all other metallic impurities are reduced to tolerable levels. An extraordinary separation factor of 10^{10} for yttrium from ^{90}Sr is achieved. The process uses only nitric acid and water as reagents and is simple and inexpensive.

   The efficacy of treatment of cancerous tumors with radioactive agents is markedly increased if the radioactive isotope can be delivered directly to the tumor by a monoclonal antibody which can recognize and bind to antigens present on the surfaces of the tumor. The effects of the radionuclide are concentrated on the tumor rather than throughout the entire host. ^{90}Y, with a half-life of 64 hours, exhibits chemistry suitable for this application. Zirconium (Zr), a decay product of yttrium, is a major competitor for the site on the monoclonal antibody. Significantly, the new separation process produces ^{90}Y with Zr levels that offer no interference with bonding of the radioactive ^{90}Y to monoclonal antibodies.

   The new process resulted from a collaboration between the Chemical Separations and Nuclear Medicine groups at Argonne National Laboratory. The fundamental research basic to development of both the SREX and TRUEX processes was supported by the Division of Chemical Sciences, while the Division of Nuclear Energy supports the Isotope Production and Distribution activities at Argonne National Laboratory.

2. ***Organometallic Reactions Conducted in Liquid Xenon***

   A liquified noble gas, xenon, has been used for the first time as a solvent for preparative reaction chemistry by chemists at Lawrence Berkeley Laboratory (LBL). Xenon, which exists as a liquid at modest pressures (2-9atm) in the temperature range from 100C to -60C, has been successfully used as an inert solvent for preparative C-H oxidative addition reactions.

   The LBL group had previously found an iridium complex that, when irradiated with UV light, reacted with all C-H bonds to which it was exposed. This ubiquitous activity posed a serious problem because it prevented the use of common organic solvents for important alkane activation studies, such as the investigation of C-H insertion in organic substrates, thus restricting the applicability of the unique reaction. The new solvent system has now allowed the chemists to carry out the activation of several new substrates and to demonstrate for the first time that alkane C-H oxidative addition can occur with a tertiary C-H bond. Alcohols were found to undergo apparent insertion at either their C-H or O-H bonds. The reaction of the iridium complex with methane represents the first generation of the metal methyl hydride under kinetically controlled conditions.

Although liquified noble gases have been used as solvents in various spectroscopic investigations, they had not previously been employed for preparative chemistry. Work is continuing on C-H insertion reactions of other substrates that cannot be easily liquified, using liquid xenon in fast kinetics experiments, and determining the cause of the dramatic substrate and solvent effects with alcohols. These important results enlarge the scope of our understanding of the metal catalyzed reactions of alkanes, originally discovered independently by Professors Bergman at the University of California, Berkeley, and W. A. Graham at Alberta, and may advance the catalysis of methane conversion to liquid fuels and chemicals, a high priority BES research area of opportunity.

3. ***New Molecular Models for Photosynthesis***

A series of structurally rigid, three-part molecules has been synthesized and found to duplicate for the first time the high ion pair yield, the charge separation lifetime, and the structural characteristics of the light-energy conversion apparatus of photosynthesis in the solid state. Up until now, no such model system has been made to function in the solid state at any temperature. The research, led by Dr. Michael Wasielewski of Argonne National Laboratory, involves molecules comprised of an electron donor, such as phenylenediamine or chlorophyll, and an electron acceptor, a quinone, rigidly attached to a central porphyrin in a linear array. Illumination of these molecules with visible light initiates sequential 5 and 500 picosecond electron transfer reactions which separate and store charge at opposite ends of the molecule. The charge separation lasts for 4 milliseconds, more than 10 times longer than in previously reported models. The resultant charge separated molecules are spin polarized and exhibit for the first time the electron spin resonance signal seen to date only in active photosynthetic organisms. This signal is highly sensitive to both the distance and orientation of the electron donors and acceptors within these molecules and, thus, is an excellent probe of molecular structure. The spin polarization in the solid state demonstrates that the charge separation and storage process is highly optimized. The new molecules represent an important step forward in "tuning" the geometry of model systems to the highly efficient natural photosynthetic apparatus and to the development of the concepts needed for efficient solar photochemical energy conversion.

4. ***Argonne Scientists Confirm Metal Cluster Isomers***

Scientists at Argonne National Laboratory have recently shown that bimodal chemical behavior of Nb_{12} clusters has its origins in the existence of two different isomers, that is, two structural forms of the clusters. Metal clusters afford a unique means for the study of the relationship between the structure of a surface and the chemical reactions that can occur on that surface. Because many of the catalytic processes associated with energy production and use occur at metal surfaces, studies of metal clusters may produce new concepts in catalysis with important energy implications. The significant feature of clusters that makes them so valuable for scientific studies is the variation in their structure with the number of atoms in the cluster. Scientists have known for some time that certain clusters consisting of specific numbers of atoms, so-called magic numbers, have enhanced chemical reactivity. More recently scientists have found evidence that some clusters, in particular clusters of niobium containing 12 atoms, exhibit bimodal behavior; that is, clusters of the same size react chemically at two different rates. These scientists then went on to suggest that the bimodal behavior was due to two different structures for Nb_{12}. Now, the Argonne researchers have obtained direct experimental evidence that the Nb_{12} clusters do indeed exist in two forms. They compared the photoionization efficiency of these clusters with their chemical reactivity toward deuterium molecules. The photoionization efficiency is obtained from measurements of the number of metal ions produced by laser irradiation as a function of the radiation wavelength. Because the photoionization efficiency is a property of the entire cluster and its structure, changes in the measured photoionization efficiency as the more reactive clusters reacted demonstrated that the two chemical reaction rates were associated with two distinct structures. Studies such as these relating chemical reactivity to surface structure will provide a scientific basis for the design of new catalysts.

A sizable fraction of Chemical Sciences research depends on the special facilities at DOE's national laboratories -- the Combustion Research Facility with its unique laser beam experimental and diagnostic capabilities; the Stanford Synchrotron Radiation Laboratory and the National Synchrotron Light Source which provide high intensity x-ray and ultraviolet radiation for inducing specific chemical reactions and for probing structures at the molecular level and below; and accelerators which provide beams of electrons, ions, and neutral species at intensities and in energy ranges needed to carry out a variety of chemical investigations.

About one-third of the Chemical Sciences operating budget for FY 1991 supports facility operations and nearly thirty percent directly supports research at universities. At the DOE laboratories, interactions between basic researchers and research and development teams working in energy technology areas are encouraged. National laboratory scientists also interact with research workers in the private sector, such as the automotive and petroleum industries.

Coordination between basic researchers supported by Chemical Sciences and the scientists in the energy technology programs and industry is encouraged. Various conferences and committees, e.g., the Solar Photochemistry Research Conferences, Catalysis Research Meetings, and the Hydrogen Energy Coordinating Committee, identify research needs and opportunities, compare results, and coordinate activities within DOE and with the rest of the scientific community. Reports such as those from the National Academy of Sciences/National Research Council, DOE advisory committees, and workshops also are used to identify research needs. In addition, Chemical Sciences staff members serve as advisors to energy technology activities and visit and review them at the DOE national laboratories.

Additional detailed information on the Chemical Sciences subprogram can be obtained from Robert S. Marianelli, Director, Division of Chemical Sciences, ER-14, Office of Basic Energy Sciences, Department of Energy, Washington, D.C. 20585, (301) 353-5804. A detailed summary of current projects is published annually. The most recent (August 1990) is entitled "Summaries of FY 1990 Research in the Chemical Sciences" (DOE/ER-0144/8).

Applied Mathematical Sciences

The objectives of the Applied Mathematical Sciences (AMS) subprogram are to advance the knowledge of mathematical, computational, and computer sciences required for understanding complex physical, biological, and chemical energy systems to meet both the immediate needs for supercomputer access by the research programs supported by the Department's Office of Energy Research (ER) and also the long-range computational research needs of the Department.

The AMS subprogram, managed by the Scientific Computing Staff, is divided into two ongoing activities: (1) Mathematical Sciences Research; and (2) Energy Sciences Advanced Computation.

Scientific advances traditionally have depended on experiments for data and on theory for understanding. Today there exists a third and equally important component of scientific research: computational science. Computational science is both a tool for studying the effect of control parameters on physical systems through simulations and a tool for extending the theoretical understanding and interpreting experimental data. The emergence of computational science as an important element in scientific research and technology development has been brought about by our increasing ability to do realistic modeling of physical problems and by the enormous power of high performance computing and communications.

The primary objective of the Mathematical Sciences Research (MSR) activity is to advance our understanding of the fundamental concepts of computational science, mathematics, and computer science. These concepts underlie the complex mathematical models of key physical processes encountered in the research and development programs of energy systems. The three major categories of MSR supported at the national laboratories, universities, and at private research institutions are Analytical and Numerical Methods, Information Analysis Techniques, and Advanced Computing Concepts. The emphasis in each case is to advance high performance computing and new parallel-multiprocessor architectures. This activity also established several computing research laboratories or centers to explore new concepts in large-scale scientific computing.

The Energy Sciences Advanced Computation (ESAC) activity provides access to scientific high performance computing resources and the high capacity networks required by ER investigators. The Energy Research Supercomputer Center (NERSC), formerly the Magnetic Fusion Energy Computational Center, now operates a CRAY X-MP (two processors and 2 million words of memory), the serial #1 CRAY-2 (four processors with 62 million words of memory), a CRAY-2 (four processors and 128 million words of memory), and a unique eight-processor CRAY-2 (128 million words of memory). The operating system used at NERSC is UNICOS. In 1992 the first CRAY-3 will be delivered to NERSC and two of the older machines will be retired. The NERSC Common File System has a capacity of more than three Terabytes (million million bytes) of storage. The Supercomputer Computations Research Institute at Florida State University (FSU), initiated at the direction of Congress in 1985, now operates a CRAY Y-MP (four processors with 32 million words of memory), associated Solid State Disk (128 million words), and more than 24 billion bytes of mass storage using UNICOS. FSU also has a 65,536 node Connection Machine (CM-2) with 2 billion bytes of central memory and 2,000 64-bit floating point processors.

Access to these systems is provided through the Energy Sciences Network (ESNet), a nationwide data communications computer network with international connections to Europe and the Orient. The ESNet provides widespread access to the ER-supported high performance computer resources, facilitates remote access to the major ER experimental facilities, and supports information exchange and dissemination among scientific collaborators throughout all ER programs. The ESNet is a 19 node backbone network which operates at T1 speed (1.54 million bytes per second). In 1992 ESNet will begin upgrades to T3 rates (45 million bytes per second). The ESNet is also a major component of the interagency National Research and Education Network, which ties together eight individual agency research network activities with the university research and education community through the Internet networking technology.

In FY 1992 the Scientific Computing Staff will be responsible for the Department of Energy's component of the new Federal initiative involving seven agencies, the five-year National High Performance Computing and Communications Program (HPCCP). The goals of the HPCCP are to extend the U.S. technological leadership in high performance computing and communications; to improve the U.S. productivity and industrial competitiveness; and to speed the pace of innovation to serve the national economy, national security, and the global environment. The strategy of the HPCCP is to accomplish these goals by supporting the solution to important scientific and technological challenges through a vigorous R&D effort; by reducing the risk of industrial R&D and utilizing the HPCC technologies through increased cooperation between government, industry and universities; support the underlying research, network, and computational infrastructures on which U.S. HPCCP is based; and by supporting the U.S. human resource base to meet the needs of industry, universities, and government.

Major emphasis of the new DOE HPCCP will be: (1) to enable Grand Challenge computational advances within the DOE missions by advancing software technology, by developing new algorithms that make effective use of new computer systems, and by establishing High Performance Computing Research Centers; (2) to support Gigabit R&D to enhance the ESNet and its integration into the National Research and Education Network; (3) to support fundamental research, participation by young scientists and engineers, and education at all levels; and (4) to promote R&D on new computer systems and evaluate their effectiveness on DOE problems. The earmark of the effort will be to build upon the underlying philosophy of the present AMS program: collaboration of interdisciplinary groups of scientists and engineers at the national laboratories, universities, and industry.

Some early support of the ER Grand Challenges in the philosophy of the HPCCP program was initiated in FY 1991. The projects include: Computer Design of Catalysts (Sandia-Albuquerque), Parallel Algorithms for Quantum Chemistry (Sandia-Livermore in conjunction with U.S. industry), Lattice Gas Algorithms for Porous Flow Phenomena (Los Alamos National Laboratory in conjunction with U.S. industry), Computational Materials Sciences (Oak Ridge National Laboratory, Brookhaven National Laboratory, Ames), and Environmental Remediation Computations (Oak Ridge National Laboratory, Brookhaven National Laboratory, Rice University, SUNY-Stony Brook, Wyoming, and South Carolina).

Examples of research accomplishments this past year include:

1. ***Shock Generation in Gases of Discrete Particles with Short Range Repulsive Forces***

   John von Neumann proposed a discrete particle model to simulate the flow of a gas in a shock tube in the 1940's. He conjectured that in the infinite particle-finite mass limit, solutions of this system would converge weakly to solutions of classical gas dynamics with an equation of state derivable from the interparticle force laws for the discrete system. Over the years this problem has stimulated considerable interest: Peter Lax and coauthors have recently amassed computational evidence that the von Neumann conjecture was incorrect; the solutions weakly converge to solutions of the gas dynamics equations, but the resulting equation of state was not derivable from the interparticle force law describing the discrete system. Professor James Greenberg at the University of Maryland at Baltimore has resolved the issue with proof that the amassed evidence is indeed correct. This result raises a fundamental question about the use of the thermodynamic equation of state, which normally is derived for a system in equilibrium, to describe dynamical processes far away from equilibrium.

2. ***Controlling Chaos***

   Chaos has been the subject of intense study in the last few years: it is now recognized that chaos does not mean that chaotic systems are nondeterministic, not fluctuating without rules. In groundbreaking research at the University of Maryland, Professors Celso Grebogi and James Yorke observed that deterministic chaotic systems do not have strongly resonant frequencies but can respond to guiding signals which may breach a number of frequencies. This idea has now been verified by experimental studies at the Naval Surface Weapons Laboratory and at the Naval Research Laboratory. This advance has very significant and far-reaching consequences. Most industrial processes, such as materials synthesis, are chaotic in nature and have been considered uncontrollable. This area can now be expected to rapidly develop with improved energy saving processes a likely result.

3. ***Heterogeneous Network Computing***

   Heterogeneous networks of computers are becoming commonplace in high-performance computing. Today, systems ranging from workstations to supercomputers are linked together by high speed networks. Until recently each computing resource on the network remained a separate unit, but now 20-30 institutions worldwide are writing and running truly heterogeneous programs utilizing multiple computer systems to solve applications through the use of PVM, a software package originally developed at Oak

Ridge National Laboratory. PVM (Parallel Virtual Machine) uses a network of heterogeneous parallel and serial computers as a unified computational resource, a metacomputer. Such flexibility allows different subtasks of a heterogeneous application to exploit particular strengths of individual machines on the network.

One of the DOE Computational Grand Challenges, the calculation of the electronic structure of superconductors, has been modified to run using PVM. Initially a heterogeneous network of workstations was used to achieve execution rates exceeding 250 Mflops. The performance is comparable to the performance of this application on a single processor of a CRAY YMP. More recently, a set of experiments designed to show the capability of PVM to connect several supercomputers together also used this Grand Challenge code. In one test, an Intel iPSC/860, a CRAY XMP, and an IBM RS/6000 were configured into a metacomputer. In another test, two CRAY YMP/8's and a CRAY YMP/2 were configured into a metacomputer. CRAY Research recently reported achieving 9.6 Gflops using PVM on a network of CRAY YMP computers. PVM is quickly bringing heterogeneous network computing of age.

4. ***Study of C(60) Buckyballs and Carbon Clusters***

Emerging as a new phase of carbon with a range of structural and chemical properties intermediate between small molecules and bulk phases, carbon clusters have received considerable attention over the past decade. The recent breakthrough in C(60) clusters (known as Buckminster Fullerene or Buckyballs) synthesis has particularly stimulated computational physicists and chemists to attempt realistic computer simulations to better understand the experimental measurements. Classical simulations are not accurate enough to provide reliable answers while ab-initio techniques are presently impractical for many interesting and important problems which require larger numbers of atoms and long simulation periods. The tight-binding molecular dynamics (TBMD) technique recently developed at Ames Laboratory provides a scheme for realistic simulation studies since it is more accurate than classical potentials and yet much faster than ab-initio techniques.

Using this newly developed technique, the structural, vibrational, and electronic properties of the C(60) buckyball were studied. The simulation results are in good agreement with experimental data, confirming that the TBMD scheme is accurate and reliable. In the simulation, C(60) buckyball formation is observed by cooling and compressing 60 carbon atoms from the gas phase. The buckyball was found to be stable up to temperatures as high as 5000K. The structural trend of the carbon cluster C(n) ranging from n=2 to 60 was also studied. For the larger clusters ($n \geq 18$), the ground state geometries are determined by annealing and compressing carbon atoms from the gas phase in a spherical cavity rather than just simply relaxing certain particularly chosen geometries. The simulation establishes a structural trend as the cluster size growth from n=2 to 60. In particular, there is a transition from one-dimensional linear and cyclic structures to two-dimensional cage structures as the number of carbon atoms reach n=20.

More information on the AMS subprogram can be obtained from David B. Nelson, Director, Scientific Computing Staff, ER-7, Office of Energy Research, Department of Energy, Washington, D.C. 20585, (301) 353-5800. A summary of current projects is published biannually. The most recent is entitled "Summaries of the FY 1989 Applied Mathematical Sciences Research Program", DOE/ER 0422, September 1989.

Engineering and Geosciences

The Engineering and Geosciences subprogram conducts fundamental research for DOE in these fields. The broader aspects of program design and emphasis are established through extensive interaction with the scientific and technological communities in the fields of interest, utilizing studies by the Basic Energy Sciences Advisory Committee, the Secretary of Energy Advisory Board, panels and committees of the National Research Council (NAS/NAE), specially convened workshops and individual interactions with scientists and engineers from universities, Federal laboratories, industry, and related Federal programs.

Engineering Research

The Engineering Research activity provides support for strengthening the foundations of energy related engineering practice. It accomplishes that goal by sponsoring research at universities, national laboratories, and in the private sector. With its emphasis on the more academic side of engineering research efforts, it provides support for graduate and postgraduate studies aimed at long-term energy needs, while furthering advanced engineering education. Where appropriate, university researchers are actively encouraged to collaborate with colleagues in national laboratories. As mentioned above, this program supports relevant basic engineering research in the private sector. Here the standards of achievement are identical with those elsewhere in the program with the added benefit of facilitating technology transfer.

In seeking to strengthen the foundations of engineering, the Engineering Research Program aims at two objectives: (1) to broaden the technical and conceptual base for solving future engineering problems in the energy technologies by introducing advances in basic sciences (mathematics, physics, chemistry and biology) to the mainstream of engineering practice; and (2) to extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality.

The program focuses on three interdisciplinary areas: Mechanical Sciences, Control Systems and Instrumentation, and Engineering Analysis. Topics of current interest include, but are not limited to, multiphase flows, chemical process control including bioprocessing of fuels and energy related wastes, fundamentals of intelligent systems, process plasma diagnostics and control, fracture mechanics in homogeneous materials, high critical temperature superconducting devices, optics, and engineering aspects of nonlinear systems dynamics.

While Engineering Research activities are aimed at long-term goals, important discoveries and applications sometimes emerge surprisingly early. Several successful accomplishments recently have included: (1) Direct observation has been made of apparent critical point opalescence of electrons undergoing normal-to-superconducting (and reverse) transition in high, critical temperature superconductors. This opalescence was associated universally with the increase of the level of fluctuations at the critical point. This experiment was non-trivial because the light photons were more energetic than the binding energy of the paired superconducting electrons. This appears to be the first measurement of its kind, and further study is underway to determine if the technique can be applied to other cases where electrons in solids appear to undergo a phase change; (2) Accurate gas temperatures and flow velocities in thermal plasma jets have been obtained from high resolution of the line shapes of scattered laser light. Since the results were not based on the assumption of local thermodynamical equilibrium, they can be used to test various models of plasma behavior as well as to calibrate measurements obtained by other techniques. Such diagnostics are critical in developing methods for the effective control of partial plasma deposition processes; and (3) Driven by a source of sound at the upper limit of the hearing range, a stable, repetitive emission of photon bursts has been recently observed. In the experiment, sonoluminescent pulses were emitted at a rate which coincided with the driving sound frequency. The medium was a 25% water solution of glycerine. The light, visible with the naked eye, was blue-green (about 0.5 μ) and emerged from a well-defined region in space, less than 10 μ diameter. The pulse length was about 100 times shorter than spontaneous emission time. Although there are other possible explanations, the small size of the emitting region, and the short pulse length suggest the possibility of coherent emission. While sonoluminescence is not entirely new, this appears to be the first time that the phenomenon has been produced in a reproducible, controllable experiment, thereby permitting it to be characterized in some detail. Possible patents are under consideration.

Recent important results achieved by longer term research efforts include the following examples.

1. ***Improved Understanding of the Behavior of Surface Cracks***

   One of the major outstanding problems in the area of engineering fracture mechanics is the assessment of the structural integrity of a plate or shell structure containing a crack penetrating only part way through the thickness. The solution of this problem is important in monitoring the safety and reliability of aging nuclear reactors, and power and chemical plants, as well as in the optimal design of future structural systems. Recently, researchers at the Massachusetts Institute of Technology have developed methods for analyzing ductile crack initiation, growth, and instability and have calculated the crack front stress and deformation fields. Their results on surface crack behavior are being correlated with experimental observations being conducted at the Idaho National Engineering Laboratory.

   Recently, significant progress has been achieved in understanding the complex three-dimensional aspects of elastic-plastic fracture behavior of part-through surface cracks. This was accomplished by developing and applying a two-parameter description of the crack front fields to replace the conventional one-parameter model. The amplitude of the crack tip deformation was characterized by the J-integral or the crack tip opening displacement, while the hydrostatic constraint in the near-tip region was correlated with a second parameter related to the so-called T-stress, or the second elastic Williams' eigenfunction.

   Simplified engineering applications of surface crack analysis are being developed by employing the concept of the line-spring model. Specific enhancements have included improved elastic-plastic procedures for the important case of shallow surface cracks, and simplified methods for calculating the T-stresses along surface crack fronts.

2. ***Stochastic Transport Methods Applied to the Cloud-Radiation Interaction Problem***

   A recently developed theory of radiative transfer in random media important to such applications as effectiveness of insulation has been applied to the study of cloud-radiation interactions in general circulation models of direct interest to the global change community. The clouds and clear atmosphere were treated as a two-component stochastic mixture. Using asymptotic techniques, a renormalized equation of transfer was derived which involved effective opacities to account for the stochastic nature of the atmosphere. To complete the model, the mean size and spacing of clouds, and the radiative properties of pure clouds and clear atmosphere were provided by cloud physics. Calculations were performed for the cases of a clear atmosphere, complete cloud cover, and homogenization of a partial cloud cover and clear atmosphere using simple volume weighing. The renormalized equation effectively interpolated between the two extremes by accounting for a finite correlation length in a simple way.

Geosciences

Geosciences Research objectives include development of a knowledge base for predicting the behavior and response of geologic materials such as rocks, minerals, and fluids, and the broader earth-sun system, to natural processes.

Some practical objectives to which the fundamental studies contribute include:

- *Enhanced oil and gas recovery;*
- *Environmental restoration;*
- *Geothermal reservoir lifetime analysis; and*
- *Nuclear and hazardous waste disposal*

through taking advantage of:

- *Improved understanding of fracture characteristics, heterogeneity and anisotropy important in fluid movement in geologic formations and reservoirs;*
- *Strengthened capabilities for indirect characterization and monitoring of geologic structures and in situ properties of rock masses; and*
- *Better knowledge of fundamental properties of rocks, minerals, and geologic fluids used in developing new processes and techniques for environmentally conscious use of energy resources.*

Rocks, Minerals, and Fluids

An integrating theme for the research is the interaction of rocks and minerals with geologic fluids (oil, gas, water, steam, brine, and magma) to change the geophysical and geochemical properties of both the rocks and the fluids. The scope of this program element is such as to emphasize dynamic aspects of active processes and to encompass physical, chemical, and mechanical behavior of geologic materials.

Researchers at Oak Ridge National Laboratory have recently demonstrated a significant compositional effect on partitioning of hydrogen (H) and deuterium (D) between a solution and its coexisting vapor phase. These results are of significance in attempts to use isotopic ratios such as D/H in fluids found as inclusions trapped in minerals to estimate temperature of formation. On the basis of these data, significant errors in temperature estimates are likely unless the brine/concentration effect is explicitly considered. The effect is particularly pronounced at temperatures below 100C.

Geochemical interactions between fluids and rocks, such as discussed above, take place largely at rock and mineral surfaces exposed to fluid reaction. One way of creating reactive surfaces in minerals and rocks is by propagation and coalescence of microfractures. Knowledge of the interaction of geologic fluids with porous and fractured rocks is a key to understanding and predicting transport and fixation of radioactive and hazardous constituents, in developing a sound basis for enhancing our oil and gas production, and in treating the propagation of fractures, which may enhance or inhibit fluid transport in the accessible part of the earth. The research program involves investigators at a number of academic institutions and DOE national laboratories. During the past year researchers at Los Alamos National Laboratory have used fracturing generated by pressurized fluid injection as a source of seismic energy for imaging underground features. Scientists at Stanford and Purdue Universities have advanced our knowledge of three-dimensional fracture connectivity in sedimentary rocks. Investigators at Lawrence Berkeley Laboratory have determined the interaction of propagating microfractures with pores to evaluate pore collapse during hydrostatic compression. Researchers at the University of Wisconsin, Lawrence Livermore National Laboratory, and Sandia National Laboratories have used new techniques in the analysis of acoustic emissions to interpret thermal stress response and to provide a basis for incorporating multiple micro-failures into constitutive models for rock failure.

Geophysical Imaging

A related theme is the study of fluid-bearing rocks and reservoirs by geophysical techniques to provide a high-resolution image of reservoir structure and properties. In this case the reservoir might be a host for oil and gas resources, a waste disposal site, or one used in production of geothermal energy. Program scope emphasizes innovative approaches which will lead to improved resolution in electromagnetic and seismic methods of data collection, analysis and interpretation.

Innovative techniques and approaches have been developed at Los Alamos and Livermore National Laboratories in the study of nonlinear elastic wave interactions in rocks. The objective is to evaluate the possibility of generating collimated seismic energy through interaction of propagating waves of different frequencies. [Johnson, Migliori, and Shankland "Continuous wave phase detection for probing nonlinear elastic wave interactions in rocks", J. Acoust. Soc. Am., v89, p.598-603, 1991; Bonner and Wanamaker "Nonlinear acoustic effects in rocks and soils", Rev. of Prog. in Quant. Nondestructive Eval., v.9, p.1709-1713, 1990].

Fundamental Data

An important element of the program is long-term and continuing research to acquire fundamental data on geophysical and geochemical properties of natural and anthropogenically modified geologic materials. The program scope includes:

- *Thermodynamic and kinetic studies of minerals, fluids, and mineral-fluid reactions;*
- *Physical and mechanical properties of rocks and minerals at elevated pressures and temperatures; and*
- *Solar-terrestrial interactions and impact on global change.*

Studies at Pacific Northwest Laboratories (PNL) have been directed toward acquiring basic data on solar insolation and the role of aerosols in the lower troposphere and stratosphere. The rotating shadow-band radiometer provides time-series data on atmospheric absorption of solar radiation. The investigators at PNL have been requested to provide this instrumentation in support of the Kuwait Oil Field Fire Experiment (KOFFE) in Saudi Arabia. This instrumentation will also be used in the DOE Atmospheric Radiation Measurements (ARM) program, and in a variety of separate efforts for acquiring essential data for the Global Climate Change Program.

Continental Scientific Drilling Program

Predictions must be tested by observation and measurement. In the Geosciences, direct observation of materials and processes beneath the surface of the earth is based on use of drill holes to sample and interrogate the third dimension. DOE participates in the interagency (NSF, USGS, and DOE) Continental Scientific Drilling Program to achieve this access to earth's crust and to test hypotheses, models, techniques and approaches.

During this year the major activities in this program element have centered on the use of samples obtained in previous drilling episodes in Long Valley (CA) and in the Valles Caldera (NM). A relatively large effort is being undertaken in preparation for future scientific drilling at Katmai National Park (AK).

A drilling project led by DOE's Geothermal Energy Division is providing vital new data on the deep thermal regime in the central part of the Long Valley Caldera in California. As part of the Geosciences Research program in Basic Energy Sciences, this 7,500 foot hole will be deepened by 300 feet to obtain rock samples.

More detailed information on this subprogram can be obtained from J. S. Coleman, Director, Division of Engineering and Geosciences, ER-15, Office of Basic Energy Sciences, Department of Energy, Washington, D.C. 20585. Annual reports are available, as Summaries of Research in Engineering and in Geosciences, which provide more detailed and specific information.

Advanced Energy Projects

The Division of Advanced Energy Projects (AEP) administers a core subprogram and the Small Business Innovation Research (SBIR) program of the DOE. (A description of the Small Business

Innovation Research program appears on page 45). It has also, in the past, been the administrator for the Heavy Ion Fusion Accelerator Research (HIFAR) program. As a consequence of recommendations made by the Fusion Policy Advisory Committee, the HIFAR program is being transferred to the Office of Fusion Energy during FY 1991. HIFAR will be a component of that office beginning in FY 1992.

The core program of the Division of Advanced Energy Projects supports research on novel energy-related ideas. The ideas emerge either from advances in basic research or from heretofore untried approaches that warrant funding to establish feasibility. The projects involved have higher risk than those normally supported by the customary DOE technology offices related to those concepts. The high risk of an AEP project is balanced by a correspondingly high reward for the Nation's energy posture if the project is successful. The AEP program is broad-ranged and reflects present perceptions of national needs in terms of innovative technologies in energy.

An AEP project is typically supported for a period of three years. Consequently, funds are available to initiate new projects every year. At the end of its AEP funding period, each project is encouraged to attract continuation funding on its own, newly established merit. Major consideration is given to facilitate the transfer of mature AEP projects to the proper technology development program, whether in the Government or in the private sector. Projects are selected on the basis of unsolicited proposals received from researchers at universities, industrial laboratories (especially small R&D companies) and national laboratories.

A major component of the present AEP core program consists of projects that can have a large impact on future energy conservation and environmental restoration efforts. Examples of such projects include a railplug igniter for diesel engines and the development of ion-exchange resins for radioactive waste treatment. Another significant area being explored is processing and characterization of advanced materials. Projects supported in this area include a nanometer scale fabrication technique and development of a positron microscope. The Division also supports efforts in novel sources of electromagnetic radiation, such as portable x-ray lasers and new applications for microwave generators. Innovative concepts in nuclear technology and a possible approach to controlled thermonuclear fusion through the impact of accelerated clusters of heavy-water molecules with deuterated targets are also under investigation.

Research Highlights

One AEP-sponsored research project, being pursued at Stanford University, is exploring an innovative method for growing high-T_c superconducting wire-like fibers from materials that normally are characterized as brittle ceramics. The most promising approach to increasing production rates appears to be the use of high pulling rates followed by a heat-treatment step. The process under exploration uses a miniaturized laser-heated float zone process. This is the basis of a totally new system which could permit the growth of fibers of unlimited length. The key to successful utilization of these fibers is their flexibility. Recently, the Stanford University research team has made 0.1 mm diameter wires up to 14.0 cm in length which can be bent to a 5.0 cm radius of curvature. Further developments of this technology could lead to the availability of high-T_c superconducting wire suitable for motor and magnet windings.

Another project, undertaken at the University of Arizona, has identified a potentially dramatic advance for burning spilled oil at sea. The conventional method, called "in-situ burning", is the combustion of oil slicks that have been corralled into floating boom structures. These burns have produced enormous amounts of soot and black smoke, characteristic of fuel-rich mixtures. Also, they have been limited by requirements that include calm sea conditions and stringent safety considerations.

The AEP project at the University of Arizona is exploring the feasibility of a technique called "in-situ incineration", in which the collected oil is pumped directly into a floating incinerator. The researchers have achieved very good incineration at high temperatures because of extraordinarily good ventilation. Recent test burns yield soot production estimated to be approximately 1000 times less than that generated from conventional in-situ burning.

Additional information can be obtained from Walter M. Polansky, Director, Division of Advanced Energy Projects, Office of Basic Energy Sciences, ER-16, Department of Energy, Washington, D.C. 20585, (301) 353-5995.

A report of ongoing projects, "Advanced Energy Projects FY 1991 Research Summaries", DOE/ER-0498T, September 1991, is available.

Energy Biosciences

The principal objective of the Energy Biosciences subprogram is to provide basic information and conceptual understanding in the microbiological and botanical sciences. This knowledge is critical to DOE's effort in meeting the Nation's long-term energy goals. Examples include renewable resource production of fuels and chemicals, microbiological transformation of organic and inorganic substances into useful or benign materials, biological systems for resource recovery, waste minimalization and waste management. The research is aimed at gaining an understanding of the underlying mechanisms of green plant productivity by solar energy transformation, conversion of biomass and other organic materials into fuels and chemicals by novel and improved methods of fermentation, and developing biotechnologies capable of saving energy.

Energy Biosciences research is focused on understanding the fundamental basis of the limits of productivity in green plants, how plants adapt to suboptimal conditions of growth, such as those encountered in marginal lands and waters, and the mechanisms of microbial conversion of various biomass forms. In particular, the research focuses on the biochemical pathways and their genetic and biochemical regulation relating to the utilization of abundant materials such as cellulose, hemicelluloses, and lignins and the conversion of these materials to fuels or chemicals. These studies are intended to form the basis for the future development of energy-related biotechnologies.

Microorganisms that grow in the absence of oxygen and are able to carry out fermentations with high efficiency are of special interest, as are thermophilic microorganisms, those having optimal growth and conversion rates at high temperatures. An integral part of the subprogram is the development of genetic information that may ultimately be used to produce new or improved microorganisms and plants that can be used to facilitate the production of fuels or petroleum-conserving chemicals or be used for new biotechnologies capable of conserving energy.

In 1987 the Energy Biosciences subprogram became involved in a multiple Federal agency effort to encourage plant-related research in the U.S. This has led to the establishment of several research centers in the U.S. whose goals are to address specific plant research areas. The Energy Biosciences subprogram is funding a center at the University of Georgia concentrating on the structure and function of complex carbohydrates of plants and microbes. The program also funds a center at Arizona State University that is focused on employing site-directed mutagenesis for producing mutants with defined protein changes to study the early biochemical and biophysical events in photosynthetic capture and conversion of light energy.

Recent Energy Biosciences accomplishments include:

1. ***Photosystem I Deficient Mutants***

   Three independent studies performed at three university-based laboratories offer the potential of dissecting the two photosystems of photosynthesis. Photosystem I has not been addressable using physiological or biochemical genetics as no mutations deficient in photosystem I have been isolated in organisms where modern molecular biological techniques can be readily applied. A recent discovery by Dr. Lee McIntosh (Michigan State University) has shown that a transformable unicellular organism, *Synechocystis*, can grow in the dark (i.e. without photosynthesis) provided that five minutes of blue-light are provided each day. This will permit the isolation of photosystem I lacking mutants, and their subsequent molecular analysis. Another cyanobacterium, the filamentous *Anabaena*, can also grow without photosynthesis and is amenable to molecular genetic manipulation. Dr. Peter Wolk, also of Michigan State University, is responsible for directing this work. Dr. Lawrence Bogorad (Harvard University) has isolated a mutant of *Synechocystis* that is killed by high light intensities. This particular mutant can be exploited to develop a screening strategy for the ready isolation of photosynthetic mutations.

2. ***Mechanisms of Fungal Toxin Resistance***

Host-selective fungal toxins have proven agriculturally devastating in two recent epidemics. Although several such toxins are known, the biosynthetic apparatus for their synthesis and the basis of their host-selectivity were both unknown. Recently, Dr. Jonathan Walton and coworkers (Michigan State University) succeeded in cloning the sequence of DNA that is responsible for the biosynthesis of the toxin produced by a fungal corn pathogen. The group also has identified the mechanism by which certain corn plants are resistant to the toxin. Genetic crosses giving both susceptible and resistant corn plants were analyzed for the capacity of the plant to metabolize the toxin. There was a strict correlation between the inability to detoxify the toxin and susceptibility. Although detoxification as a mechanism of resistance to antibiotics and herbicides is well known, this is the first time that detoxification has been clearly demonstrated to play a role in plant pathology.

3. ***Patent Awarded for Ethanol-Producing Bacterium***

On March 19, a ceremony was held at the Department of Commerce to commemorate the awarding of the five-millionth patent by the U.S. Patent Office. The patent awarded to the University of Florida concerns the genetic engineering of bacteria in order to extend the variety of substrates that can be used in the biological production of ethanol. The organism used, *E. coli*, has the major flow of carbon altered such that ethanol instead of acetate and carbon dioxide is the major product. Thus, the metabolic capacities of *E. coli* to use numerous growth substrates has been combined with the ability to synthesize significant levels of ethanol. The invention is based on the fundamental research conducted by Dr. Lonnie O. Ingram on the ethanol-producing bacterium, *Zymomonas*. This research is a prime example of the role of basic research in leading to biotechnological advances for U.S. industries.

4. ***Bioremediation Technologies***

The white rot fungus, *Phanerochaete chrysosporium*, has been studied for a number of years for its ability to degrade plant lignins. As lignin is a polymer of aromatic compounds and the initial lignin degradative steps are relatively nonspecific, Dr. Michael Gold of the Oregon Graduate Institute of Science and Technology pursued studies on the ability of the organism to degrade aromatic pollutants. The fungus was found to readily degrade such pollutants as 2,4-dichlorophenol, a man-made compound that is a serious contaminant in certain instances. The pathway of degradation was discovered to involve an oxidation by lignin or manganese peroxidase followed by several novel reduction and methylation reactions. As a result of these investigations, this organism is now being integrated into the full range of bioremediation processes available for pollution control and waste management.

Further information can be obtained from Robert Rabson, Director, Division of Energy Biosciences, ER-17, Office of Basic Energy Sciences, Department of Energy, Washington, D.C. 20585, (301) 353-2873. Also available is the "Annual Report and Summaries of FY 1990 Activities," DOE/ER-0469P, September 1990, which includes detailed descriptions of ongoing activities.

Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program, which is mandated by the Small Business Innovation Development Act of l982 (P.L. 97-219), supports research and R&D activities at small business enterprises. DOE's SBIR program is administered through the Division of Advanced Energy Projects in the Office of Basic Energy Sciences within the Office of Energy Research.

The principal objectives of the SBIR program are: to stimulate technological innovation; to use small business to meet Federal R&D needs; to foster and encourage participation by minority and disadvantaged persons in technological innovation; and to increase private sector commercialization innovations derived from Federal R&D. The Department's SBIR program supports high-quality research or R&D grant applications on advanced concepts relevant to important energy-related scientific or engineering problems and opportunities that could lead to significant public benefit if the research is successful.

As prescribed in the legislation, the SBIR program is designed for implementation in a three-phase process, with Phase I determining, insofar as possible, the scientific or technical merit and feasibility of ideas proposed for investigation. The period of performance in this initial phase is relatively brief, typically about 6 months, and the awards are limited to $50,000. Between one-third and one-half of the Phase I projects can be expected to proceed successfully into Phase II, the principal research or R&D effort, in which qualified projects can receive awards as high as $500,000 for periods of up to 2 years. In Phase III, small businesses carry out the commercial application of the research or R&D effort with non-Federal capital or, alternatively, Phase III may involve follow-on non-SBIR Federal contracts for products or services desired by the Government.

The total Department funding amounts provided for SBIR projects are in accord with the requirements of P.L. 97-219 as amended, which specifies that the 11 agencies subject to this law (including DOE) spend certain percentages of their extramural research or R&D funds on SBIR projects. The law specifies 1.25% for each fiscal year from 1986 through 1993. On this basis, the DOE budget for SBIR is approximately $39 million in FY 1991. The budget for DOE's Defense Programs is exempt from participation in SBIR.

The Department issues SBIR program solicitations annually, with research or R&D opportunities provided each year in about 30 topical areas. The slate of topics changes somewhat from year to year, so as to offer, in time, a dynamic representation of DOE's wide range of interests in non-defense research related to its mission. Topics in recent solicitations covered the areas of Basic Energy Sciences, Health and Environmental Research, High Energy and Nuclear Physics, Magnetic Fusion Energy, Conservation and Renewable Energy, Nuclear Energy, and Fossil Energy.

In the first 8 years of the program, 1983-1990, 9,030 Phase I proposals were received and 984 Phase I awards were made. Three hundred seventy-two Phase II awards were made through FY 1990. The award selections have been made on the basis of scientific and technical excellence of the proposals.

The Department continues to receive reports of Phase II projects that are achieving success in Phase III. For example, a Phase II award was made in 1988 to Advanced Technology Materials Inc., a high-technology firm based in New Milford, CT. This award has already resulted in the development of a device for removing key contaminants from gases used in the chemical vapor deposition of solar cells and semiconductors. The device earned the company a 1988 R&D-100 Award, and has already become an industry standard. For 1990, sales of this product amounted to $7 million. Investments in the company to develop the product have reached about $6 million.

Another Phase II awardee, National Recovery Technologies, Inc. (NRT), of Nashville, TN, has received $12 million in sales for a municipal solid waste materials recovery process that removes

80% of the glass, aluminum, and ferrous metals from the waste stream prior to combustion. Key benefits of the NRT system include a 33% reduction in ash production, a 38% increase in incinerator capacity, a 20% increase in boiler efficiency, and the ability to provide municipalities with a more comprehensive solid waste disposal solution. NRT also received $3.4 million in venture capital investment to commercialize the project. Systems have been sold to municipalities in West Germany, Italy, Canada, Florida, Illinois, Kentucky, New Jersey, New York, Ohio, Pennsylvania, Texas, and Wisconsin.

Additional information about the SBIR program is available from Samuel J. Barish, SBIR Program Manager, ER-16, Department of Energy, Washington, D.C. 20585, (301) 353-3054. Reports containing abstracts of the projects receiving support are available. The current reports are "Abstracts of Phase I Awards, 1990, DOE/ER-0472" and "Abstracts of Phase II Awards, 1990, DOE/ER-0467". The most recent program solicitation can be obtained by contacting the SBIR Program Manager.

Major BES Facilities

__*High Flux Beam Reactor*__
Brookhaven National Laboratory, Upton, New York

The High Flux Beam Reactor (HFBR) produces high-intensity neutron beams used for research in many areas of science. Neutrons are used to irradiate materials, to make them radioactive, or to transmute one element into another. They also are used as probes by nuclear and solid-state physicists, chemists, and biologists. How neutrons are scattered by molecular structures provides a means of determining those structures and some of their properties. Neutron scattering techniques yield information on the fundamental properties and behavior of materials and chemical and biological substances which cannot be obtained by any other means. The HFBR is one of two high-flux research reactors supported by DOE, both of which are world-class research reactors for neutron research.

Current research using the HFBR includes studies of:

- *The structure and dynamics of magnetic materials;*
- *The dynamics of materials as they change phase;*
- *Neutron irradiation effects on the physical properties of materials;*
- *The molecular structure and dynamics of organo-metallics;*
- *Small-angle neutron scattering of biological substances -- small-angle scattering is a refinement providing more precise information on highly complex structures;*
- *Lattice structure and dynamics in condensed matter systems;*
- *Amorphous materials -- short-range order and excitations; and*
- *The neutron spectroscopy of low-lying excited states in solids.*

The HFBR, which cost $12.5 million to build, went critical in 1965 and attained full power in 1966. Originally 40 MW, its power was increased to 60 MW in 1982. The reactor has a maximum thermal neutron flux of 1.1 x 10^{15} neutrons/cm^2-sec available for research. Use of the HFBR facilities is divided between Participating Research Teams (PRT's) and general users. PRT's consist of scientists from Brookhaven National Laboratory (BNL) or other Government laboratories, universities, and industrial laboratories who have a common interest in developing and using beam facilities at the HFBR. In return for their development and management of these facilities, each PRT is assigned up to 75% of the available beam time, with the remainder being reserved for general users.

A limited amount of funding is made available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by Faculty/Student research groups performing experiments at the National Synchrotron Light Source (NSLS) or at the HFBR and is aimed at university users having only limited grant support for their research.

Experiments proposed by users are reviewed for scientific merit by a Program Advisory Committee composed of specialists in relevant disciplines from both within and outside BNL. The committee reviews the uses to be made of the facilities by the PRT's and general users and assigns priorities as required.

Several of the nine experimental beam ports at HFBR are used by more than one scattering instrument; three are used for nuclear physics research, and the rest for neutron diffraction or scattering research. The reactor can also be used to irradiate samples through any one of seven different vertical access tubes. The in-core total flux is 2.4 x 10^{15} neutrons/cm^2-sec. The building that houses the reactor and ancillary equipment has floor space for experimental apparatus. With its cold moderator facility, the HFBR provides the largest source of very low energy neutrons in the United States.

Recent accomplishments dependent on the availability of the HFBR include:

1. ***Magnetic Excitations in $YBa_2Cu_3O_{6+x}$***

   Pioneering neutron scattering investigations of magnetism in the high T_c systems have been performed at BNL beginning with La_2CuO_4, the first compound for which large single crystals became available, and continuing on Sr-doped crystals. In 1988, these studies were extended to the $YBa_2Cu_3O_{6+x}$ systems, for which the maximum superconducting transition temperature is 90 K at x = 1. Large single crystals with various oxygen contents have been grown by a group at the Institute for Molecular Science in Japan. Extensive neutron scattering measurements of magnetic excitations in these crystals have been performed in collaboration with researchers at the Massachusetts Institute of Technology. This work provided evidence for three-dimensional magnetic ordering in samples with low oxygen content, and evidence of a very strong magnetic coupling between copper atoms within the CuO_2 layers, the common structural element of these compounds. This research provided clear evidence that magnetism and superconductivity are closely associated in the layered copper oxide compounds.

2. ***Intercalation Compounds: Implications for Advanced Battery Materials***

   Neutron diffraction at the HFBR was used to determine the local distortions for lithium inserted between layers of graphite and titanium disulfide in systems of practical interest. High capacity rechargeable batteries are likely to be important in future energy strategies and this research provides new insights into the selection of materials for batteries based on "intercalation" compounds. Ions intercalated (inserted) between layered structures at high temperatures create local distortions to the structure that stabilize the distorted structure when the temperature is lowered. Many new battery technologies rely on intercalation (insertion or doping) of a mobile charge carrier (ion) into an inorganic lamellar or organic polymer electrode. This research helps demonstrate that phase transitions, which are detrimental to electrode life due to dimensional changes, can be controlled by proper selection of dopant and host material. This breakthrough provides a rational basis for selecting host materials for intercalation batteries in terms of their elastic properties. Furthermore, more recent data suggest that the same concepts may be applied to polymer electrodes.

The HFBR was unavailable for research this past year. The reactor was restarted in May 1991 and full operation is expected during the early summer 1991.

Additional information about HFBR can be obtained from David S. Rorer, HFBR - Bldg. 750, Brookhaven National Laboratory, Upton, New York 11973, (516) 282-4056.

High Flux Isotope Reactor
Oak Ridge National Laboratory
Oak Ridge, Tennessee

The High Flux Isotope Reactor (HFIR) has a high thermal neutron flux designed for production of transplutonium elements. This facility is critical to the Transplutonium Production Program of DOE. In addition to producing transplutonium elements, HFIR has four ports to permit the extraction of neutron beams from the reactor core for experimental purposes. The high flux and experimental capabilities make HFIR a unique research reactor, important not only for isotope production but also for neutron scattering, nuclear chemistry, and radiation damage research.

The HFIR cost about $15 million to build and attained its operating power of 100 MW in 1966 with a thermal flux in the target area of 2 to 5 x 10^{15} neutrons/cm^2-sec. It is a light water moderated reactor and has had an unsurpassed record of better than 90% of scheduled operation. HFIR has a unique, two-piece core, which is its fuel element; this core is about the size of a 30-gallon drum and is replaced after about 3 weeks of operation. In addition to isotope production activities and in-core irradiations, there are twelve research stations at the four experimental ports. The National Center for Small Angle Scattering Research associated with the HFIR was sponsored as a joint project of DOE and the National Science Foundation. This Center was moved to the NIST Reactor when HFIR was shutdown in 1986 for refurbishment due to radiation damage to the vessel. HFIR was restarted in early 1990 and, after a period of low-power operation, reached the new full-power level of 85 MW on May 16, 1990. The operating record since then has shown steady improvement: 37% availability during the third quarter of 1990, 61% availability during the fourth quarter of 1990, and 75% availability during the first quarter of 1991. Routine operation in the future will be at the 75% level.

The neutron scattering facilities at HFIR are used for long-range basic research on the structure and dynamics of condensed matter. Active programs are dealing with:

- *The magnetic properties of matter;*
- *Lattice dynamics;*
- *Defect-phonon interactions;*
- *Lattices in superconductors;*
- *Liquid structures; and*
- *Crystal structures.*

A wide variety of neutron scattering instruments have been constructed at HFIR. Three of these having capabilities unique within the U.S. are the "double-crystal small-angle diffractometer", the "correlation chopper", and the "wide-angle time-slicing diffractometer".

These facilities are open for use by outside scientists working on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an external review committee. Accepted experiments are generally scheduled within 6 months of the receipt of the proposal. No charges are made for the use of the beams for research to be published in the open literature, but costs of extensive use of ORNL shop or computer facilities must be borne by the user. Financial assistance is available for the travel and living expenses of users from U.S. universities. Inexperienced users will normally be able to collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full-cost recovery, including a charge for beam time.

Although the use of HFIR has changed direction over the years, with increased emphasis on neutron irradiation and beam research and radioisotope production for sales, trans-plutonium isotope production continues to be a significant effort. With the shutdown of the General Electric Test Reactor, which was a commercial supplier of a variety of radioisotopes, HFIR became the source of substantial quantities of radioisotopes for the industrial community.

Other research at HFIR is supported by the Fusion Energy and Nuclear Energy Programs, the Nuclear Regulatory Commission, and the National Science Foundation.

Recent Accomplishments from HFIR include:

1. ***Phonons In High-Temperature Superconductors***

   Triple-axis neutron spectrometry at HFIR has been used in conjunction with experiments at the Oak Ridge Electron Linear Accelerator to show that phonons are connected closely with superconductivity in the ceramic superconductors. The results show that the phonon modes for the copper atoms in the copper-oxygen planes soften dramatically at the transition temperature, while those modes propagating along the c-axis are unaffected. The neutron results have shown that a number of individual, inplane phonon modes soften and broaden at the transition temperature, particularly near the zone boundary. The fact that some phonon modes decrease in energy at the transition temperature shows that there is a direct coupling between superconductivity and certain phonon modes, namely those propagating in the copper-oxygen planes. The change in width of the mode gives an estimate of the electron-phonon coupling strength which appears to be much larger than in conventional superconductors.

Additional information about HFIR can be obtained from the Research Reactor Division, ORNL, Oak Ridge, Tennessee 37831, (615) 574-8049.

National Synchrotron Light Source
Brookhaven National Laboratory
Upton, New York

The National Synchrotron Light Source (NSLS) is a unique user-oriented facility for advanced multidisciplinary research with synchrotron radiation -- highly intense radiation emitted by relativistic electrons traveling in circular paths at very high energies. Synchrotron light from the NSLS is continuous in spectrum, pulsed, and high in intensity, with the spectral peak related to the electron energy and radius of the circular orbit. At the NSLS there are two electron storage rings, one producing vacuum ultraviolet and infrared radiation, the other producing x-rays. At NSLS, a wide-range of research techniques are used by biologists, chemists, solid-state physicists, metallurgists, and engineers for basic and applied studies. Fundamentally, these techniques involve use of synchrotron radiation to probe the structure of matter but with capabilities well beyond those of x-ray and light sources previously available. These include many traditional techniques refined and extended to meet the opportunities provided by synchrotron radiation for the study of structure and dynamics of matter. The techniques include extended x-ray absorption fine structure (EXAFS), scattering, diffraction, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, and infrared vibrational spectroscopy.

The NSLS began operating in 1981. The x-ray ring is about 170 meters in circumference. The vacuum ultraviolet (VUV) ring is 44 meters in circumference. A common injector meets the high-current requirement (1.0 A) for both rings. The VUV ring has been used routinely for research since early 1984. It operates at 750 MeV. The x-ray ring operates at 2.5 GeV. Since there are 47 ports at the two rings with each port capable of supporting one to three experiments, the NSLS has the potential of running about 100 experiments simultaneously.

Users are an important concern in operating the NSLS; the scientific community participates heavily in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines have been designed and instrumented by "Participating Research Teams" (PRT's). The PRT's are given priority for up to 75% of their beam line(s) operational time for a 3-year term.

Research groups are now in the process of forming insertion device teams (IDT's) to design and instrument beam lines and insertion devices. After an initial "commissioning period" to assure safety and reliability, NSLS and PRT beam lines will become available to general users. In the latter case, PRT's provide liaison and utilization support to general users.

Proprietary research can be performed at the NSLS, a full-cost recovery fee being charged for the amount of beam time utilized. The DOE has granted the NSLS a Class Waiver, under the terms of which proprietary users of the NSLS will have the option to retain title to inventions that result from research performed at the NSLS.

A limited amount of funding is available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program to defray expenses incurred by research groups performing experiments at the NSLS. The Faculty/Student Support program is aimed at helping university users having only limited grant support for their research.

Some applications of the interaction of synchrotron radiation with matter are:

- *Studies of the state and behavior of gases;*
- *Studies of the surfaces of solids;*
- *Studies of metal atoms in biological systems;*
- *Analysis of the atomic structure of microscopic samples;*
- *Microscopy;*
- *Research related to the miniaturization of computer chips; and*
- *Magnetic structure of surface and near surface layers in materials.*

Recent accomplishments requiring the unique capabilities of NSLS are:

1. ***Synchrotron Mossbauer Spectroscopy***

   The world's first use of direct Mossbauer spectroscopy without the need for a radioactive source of irradiation was achieved this year at NSLS. Mossbauer spectroscopy is a valuable technique for probing structures and local site geometries in solid materials. Previously, Mossbauer spectroscopy could only be performed using a radioactive source of gamma rays. This severely limited the applicability of the method because of both the care needed when working with such sources and the small number of chemical elements possessing the appropriate gamma ray emission. The accomplishment of synchrotron radiation Mossbauer spectroscopy is expected to stimulate similar experiments at synchrotrons around the world and will greatly expand the uses of the technique.

2. ***Surface-Induced Ordering of a Polymer Film Detected by X-ray Scattering***

   The first successful effort to characterize the ordering induced in bulk polymers by the presence of a surface was achieved at NSLS. Grazing incidence x-ray scattering was used to assess the polymer interchain and intrachain ordering near the surface of an aromatic polyamide with the chemical acronym, PMDA-ODA. This material is in widespread use in the microelectronics industry and is used at storage rings as a window material because of its excellent thermal and radiation stability. Films of the material also have an unusually smooth surface. The results demonstrated that the structure and conformation of the polymer near the surface is far different from the bulk morphology. The interface induces an essentially crystalline order at the polymer surface which persists only over short distances before normal liquid crystalline structure is observed. Because of the short range of the surface structure, no techniques were previously available to characterize the atomic arrangements near the surface.

The users of the NSLS facility also include industrial researchers from such Fortune 500 corporations as IBM, Exxon, Bell Laboratories, DuPont, General Electric, and Mobil. The DOE construction of NSLS provided for the building, storage rings, and a limited amount of experimental equipment for the beam lines. A substantial amount of additional instrumentation and equipment has been installed with private industry funds.

Additional information about NSLS can be obtained from Susan White-DePace, NSLS Department, Building 725B, Brookhaven National Laboratory, Upton, New York 11973, (516) 282-7114.

Stanford Synchrotron Radiation Laboratory
Stanford University
Stanford, California

Basic Energy Sciences is responsible for operating the Stanford Synchrotron Radiation Laboratory (SSRL). The SSRL is one of several national facilities, and DOE's second one for the utilization of synchrotron radiation for basic and applied research in chemistry, physics, biology, and materials science. The SSRL was expanded under the auspices of the National Science Foundation in partial response to a National Academy of Sciences report that pointed out the potential for research in the newly identified area of synchrotron radiation.

The Stanford Positron Electron Asymmetric Ring (SPEAR) has been shared with the High Energy Physics program, but has recently become dedicated for SSRL purposes, and with the new 3 GeV injector, SSRL is totally independent of High Energy Physics operations for the first time. At present, available time is heavily oversubscribed by the solid-state, chemical, and biomedical research communities for its high-intensity photons in the ultraviolet and x-ray regions of energy.

The synchrotron radiation at SSRL is produced by the 4-GeV storage ring SPEAR operated by the Stanford Linear Accelerator Center (SLAC). The SSRL is a user-oriented facility that welcomes inquiries and proposals for experiments from qualified scientists.

The SPEAR spectrum extends from the infrared through the visible, ultraviolet (UV), vacuum ultraviolet (VUV), and deep into the x-ray region. For example, in the x-ray region, SPEAR provides five orders of magnitude more continuum radiation than the most powerful conventional x-ray generators. In addition, an experimental beam line recently commissioned on the SLAC storage ring, PEP (an acronym for Positron Electron Project), which makes use of a special permanent magnet device known as an undulator, has produced the brightest x-ray source in the world.

The extraordinary properties of synchrotron radiation as a research tool have led to many very important scientific results including:

- *Development of the widely used Extended X-ray Absorption Fine Structure (EXAFS) technique as a powerful structural tool;*
- *Many advances in surface physics based on the photoemission technique, using high intensity tunable VUV radiation from 10 to 1,000 eV;*
- *Dynamic studies of conformational changes in biological systems, using time dependent x-ray diffraction and fluorescence lifetime techniques;*
- *Development of anomalous diffraction as a broadly applicable tool of crystallography;*
- *Results in other areas such as topography, lithography, and microscopy; and*
- *Development of a method of non-invasive angiography for heart disease patients.*

Recent accomplishments dependent upon the availability of the SSRL have included:

1. ***Synchrotron X-ray Studies of Growth of Semiconductor Surfaces***

   The first in situ x-ray study of the growth of a semiconductor surface by organo-metallic chemical vapor deposition was carried out at the SSRL. The study was made of the growth of zinc selenide on a gallium arsenide (001) surface using grazing incidence scattering of extremely bright x-rays produced at SSRL. Recently improved magnet technology was able to provide a "bright" enough beam of x-rays to carry out the desired experiments. These initial experiments, involving the operation of a chemical vapor deposition apparatus in the x-ray beam line, demonstrated the feasibility of using proven x-ray-based analytical techniques to "see" structural details while the films are growing. These key experiments involved a collaboration among AT&T Bell Laboratories, SSRL, and Stanford University scientists.

2. ***Two-Dimensional Compressibility of a Metal Measured for the First Time***

   Lawrence Berkeley Laboratory scientists, in a collaborative effort with investigators from IBM-Almaden and the University of Puerto Rico, measured for the first time the two-dimensional compressibility of a metal. Using a beam of x-rays at the SSRL, the structure of a lead film was observed during its deposition on a silver surface. The separation between neighboring lead atoms in the monolayer at the silver surface decreased as applied electrical potential (voltage) was raised until multilayer or bulk deposition of the lead occurred.

   The data obtained were used to calculate the two-dimensional compressibility of the monolayer (1-atom thick) lead film in contact with the silver surface. This research result and the technique used to obtain it are important for understanding thin film deposition processes and their control; such processes are widely used in fields such as electronics and corrosion resistant coatings.

Current research activities at SSRL include:

- *X-ray absorption, small and large angle scattering as well as topographic studies of atomic arrangements in complex systems such as surfaces, amorphous materials and biological materials;*
- *Soft x-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter;*
- *Non-invasive angiography; and*

- *X-ray lithography and microscopy.*

SSRL serves approximately 500 scientists from 124 institutions working on over 200 active projects. A wide variety of experimental equipment is available for the user and there are no charges either for use of the beam or for the facility-owned support equipment. Proprietary research may be performed on a cost-recovery basis by special arrangement.

SSRL has six beam lines, most with multiple experimental stations. It is a user-oriented facility which welcomes proposals for experiments from all qualified scientists. Proposals are subjected to peer review and more than half of the proposals do receive beam time.

A major transition has occurred at SSRL during the last year with the completion of a new injector and the dedication of the storage ring, SPEAR, as a synchrotron radiation light source totally independent of the SLAC high energy physics operations.

The dedicated 3 GeV injector synchrotron for the SPEAR storage ring was completed on schedule and within budget in November 1990, meeting all major design goals. It is now in the advanced stages of commissioning and the first synchrotron radiation experiments using the injector as the SPEAR source will occur in mid-summer 1991. The new injector provides SSRL's physical independence from the SLAC 2-mile long linear accelerator.

The $14 million project, funded by the Division of Materials Sciences of BES, was started in February 1988 and officially completed 33 months later, on November 29, 1990. The basic goal is a 3 GeV electron beam for injection into SPEAR which would allow SPEAR to be filled to 100 mA in less than 5 minutes.

Preparation for independent operation of SPEAR for synchrotron radiation research began in February 1991. By mid-May a maximum injection rate of 43 mA per minute was obtained at an injection energy of 2.3 GeV, demonstrating the ability to fill SPEAR to 100 mA in less than 5 minutes.

One of the goals of the injector project was to allow SPEAR to operate in a new low emittance mode. This was successfully tested in May 1991 while accumulating 85 mA of beam in the first test. The traditional emittance of SPEAR has been 510 nm-rad, while measurements in the new mode were 150 nm-rad, providing an order of magnitude increase in brightness.

More information can be obtained from K. M. Cantwell, SSRL, Bin 69, P. O. Box 4349, Stanford, California 94305, (415) 854-3300 ext. 3191.

<u>Intense Pulsed Neutron Source</u>
Argonne National Laboratory
Argonne, Illinois

The Intense Pulsed Neutron Source (IPNS) is a dedicated user-oriented facility for advanced research with pulsed neutrons; it serves the physics, materials, chemical, and life sciences research communities.

Unlike nuclear reactor sources which put out a steady flow of neutrons, this machine provides a high flux of neutrons in bursts that are precisely in step with the 30 Hz frequency (a 30 Hz frequency means there are 30 bursts per second) of the proton accelerator. High-energy protons from a proton synchrotron impinging on a heavy metal target produce bursts of neutrons knocked out of the target; these are called spallation neutrons. The resulting pulsed beams of neutrons, exploited using time-of-flight techniques, have the following characteristics:

- *High peak intensity thermal neutrons;*
- *High peak intensity epithermal neutrons; and*
- *Pulsed delivery for investigating time-dependent phenomena, such as following shock waves, heat pulses, or laser flashes.*

In materials research, pulsed neutrons can be used to study:

- *Static and dynamic properties of liquids and amorphous solids;*
- *Defects, voids, and aggregates in materials;*
- *Structure and dynamics of polymers and biological material;*

- *Magnetic, crystallographic, and electronic changes;*
- *Phonon structure and magnetic excitations in solids;*
- *Surface phenomena and superconductivity; and*
- *Radiation damage at cryogenic temperatures.*

Two principal types of scientific activity are underway at IPNS: neutron diffraction, concerned with the structural arrangement of atoms (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties; and inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level. At the same time, it is expected that the facilities will be used for fundamental materials measurements as well as for technological applications, such as to measure stress distribution in materials and characterization of zeolites, ceramics, and hydrocarbons.

The IPNS, which began operation in FY 1981, has a peak thermal flux of 3×10^{14} neutrons/cm^2-sec, a peak epithermal flux at 1 eV of 10^{15} neutrons/ cm^2-sec, and a time average fast flux of 2×10^{12} neutrons/cm^2- sec. The proton current is 8 microamps providing 500 MeV protons in 30 bursts per second of 2×10^{12} protons per burst.

Access to IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a program committee consisting of eminent scientists, mostly from outside Argonne.

The neutron scattering assembly has seven spectrometer stations, and the radiation effects assembly includes two cryostat stations for investigations at 4°K. Six additional facilities are available for special experiments with, for example, solid He^3, polarized neutrons, and ultra cold neutrons, for high-temperature irradiations, and for temperatures at less than .002°K.

The authorized construction cost for IPNS ($6.4 million) provided for beam transfer from the proton synchrotron and construction of the spallation target area. In addition, $2.4 million was provided to upgrade the experimental capability with a variety of spectrometers, detectors, and computer interfaces.

The person to contact for additional information is T. G. Worlton, Scientific Secretary, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, (312) 972-8755.

Manuel Lujan, Jr. Neutron Scattering Center, LANSCE
Los Alamos National Laboratory
Los Alamos, New Mexico

The LANSCE facility is a pulsed spallation neutron source driven by the 800-MeV Los Alamos Meson Physics (LAMPF) linear accelerator. Neutron scattering research is currently carried out at LANSCE using the advantages of time-of-flight methods and high epithermal flux. A proton storage ring (PSR) began operation in 1985 providing 12 neutron bursts per second, for the world's highest peak thermal flux, 1.7×10^{16} neutrons-cm^2/sec, for neutron scattering research. In addition, it will also be a source of epithermal neutrons many orders of magnitude larger than reactors for neutron scattering research in solid state physics, chemistry, biology, polymers, and materials science.

LANSCE will be operated as a national user facility with formal proposals for experiments reviewed by a Program Advisory Committee (PAC) to allocate two-thirds of the available beam time. The PAC will evaluate proposals on the basis of scientific excellence and optimal use of LANSCE capabilities. One-third of the neutron scattering beam time is reserved for laboratory discretionary research, research pertinent to DOE applied program goals, and instrument development. The LANSCE instrumentation is available without charge for nonproprietary research. The facility is open to all U.S. citizens and permanent resident aliens and to visits of less than 7-working days for citizens of non-sensitive countries. DOE approval is required for any other foreign national visits.

Available instruments are: (a) 32-meter neutron powder diffractometer; (b) a single crystal diffractometer based on the Laue time-of-flight technique; (c) a filter difference spectrometer for chemical and optic mode spectroscopy; (d) a constant-Q spectrometer for studies of elementary excitations in single crystals; and (e) a liquids, amorphous, and special environment diffractometer. A considerable effort is currently directed toward pulsed source instrument development including, currently, a chopper spectrometer and a low Q diffractometer.

The person to contact for information is J. Eckert, MS H805, Group P-8, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, (505) 667-6069.

Combustion Research Facility
Sandia National Laboratory
Livermore, California

The Combustion Research Facility (CRF), which cost $10.3 million to construct, provides a range of instrumentation not available in other laboratories and, thus, provides a unique capability to outside users, including many non-DOE groups, for combustion research. The focus of the laboratory is on laser diagnostics of combustion systems, but a variety of burner systems and special facilities are available, including those for research on coal combustion and internal combustion engines. The staff at CRF provides users with technical support covering such diverse fields as chemistry, fluid dynamics, computer modeling, and pure and applied spectroscopy. The CRF research staff also has the necessary scientific strengths to serve the DOE combustion program's research objectives -- maximizing the efficiency of processes while minimizing the production of undesirable pollutants. Examples of research carried on at CRF include:

- *Detection and measurement in flames of short-lived reactive intermediates in key combustion reactions;*

- *Energy transfer process and chemical kinetics of molecules of combustion interest;*

- *Laser velocimetry to study turbulence effects in an internal combustion engine; and*

- *In situ laser diagnostics of the interactions of materials surfaces with flames.*

As an example of the research conducted at the CRF, results on alcohol combustion were reported in 1989 that provided a considerable improvement in the understanding of alcohol combustion. The effectiveness of alcohol fuels in existing and new internal combustion engines is of critical concern and has prompted research on their combustion chemistry. Studies at the CRF on the reaction mechanisms of the hydroxyl radical, a dominant reactive species, with various alcohols have provided new, unanticipated information on the reactions that take place. Studies at the CRF, employing its unique capabilities to follow extremely rapid reactions under a wide range of experimental conditions, showed that the hydroxyl radical-alcohol reaction mechanism actually changes significantly with temperature. The studies were characterized by a high degree of accuracy for chemical reaction rate measurements and by the use of isotopic enrichment to sort out competing reaction mechanisms. The major surprise of the experiments was the discovery that at high temperatures, the hydroxyl radical-alcohol reaction constitutes a catalytic, chain mechanism for the conversion of alcohols to a particular class of hydrocarbons called alkenes. Thus, in modeling a practical combustion system involving alcohol fuel, the subsequent combustion chemistry of the product alkene also must be included.

Combustion scientists from other locations participate through the Visiting Scientist Program in ongoing research projects, and facilitate the transfer of fundamental combustion technology to industry and universities. Visitors come to the CRF from universities and industry to conduct research, attend meetings and short courses, and hold technical discussions with the laboratory staff.

Participants in the Visiting Scientist Program work at the facility for 2 weeks or longer. Research by these scientists is usually carried out in collaboration with members of the permanent staff; however, visitors may also bring their own experimental apparatus and take advantage of the special diagnostic capabilities available at the CRF. Sandia National Laboratory normally covers costs associated with the research program; visitors are expected to provide for their own salary and living expenses while at Livermore. Also, they are expected to publish the results of their research. Proprietary research may be done at the CRF, but only on a full-cost recovery basis.

The CRF, a building with fourteen individual research laboratories, four special laser laboratories, and a variety of support laboratories, was dedicated in March 1981. On demand, laser output can be beamed to any one of the individual research laboratories for use in a large variety of experiments.

Additional information can be obtained from P. Mattern, CRF, Sandia National Laboratory, Livermore, California 94550, (415) 422-2520.

Advanced Light Source
Lawrence Berkeley Laboratory
Berkeley, California

Under construction since 1987, the ALS is gathering momentum as it approaches its spring 1993 project completion date. ALS is the first of the third generation synchrotron radiation light sources to be constructed in the U. S. The ALS will be a high brightness, low emittance source of synchrotron radiation in the soft x-ray and vacuum ultraviolet portion of the electromagnetic spectrum. Operation and access to ALS will be similar to that for NSLS.

ALS experimental facilities are being developed in collaboration with participating research teams (PRTs). There are eight insertion-device PRTs and 6 bend-magnet PRTs, including two new bend-magnet PRTs in April 1991. Memoranda of Understanding are being negotiated with each PRT. A series of workshops to explore new scientific opportunities and to stimulate additional interest in the user community is in progress. Topics include soft x-ray lithography, photon-in/photon-out spectroscopy, circularly polarized bend-magnet radiation, and spectroscopic imaging. In addition, a workshop on industrial application of synchrotron radiation is being planned and a brochure to increase interest in the ALS from the industrial sector has been prepared and distributed.

Accomplishments related to the construction of ALS include:

1. The ALS project has moved into its building consisting of the remodelled circular building, which formerly housed the 184-inch cyclotron, and the annular addition which will accommodate the beam lines.

2. Construction of the control room has been completed.

3. The electron linear accelerator system that comprises the first stage of the ALS injector system was installed and tested. Commissioning activities began in February 1991; the first accelerated beam was achieved on February 20, 1991. The full beam energy of 50 MeV was achieved on March 6, 1991.

4. The 1.5 GeV booster synchrotron was installed in the central part of the ALS building. On May 6, 1991, ALS accelerator scientists and engineers succeeded in injecting electrons from the linac through a transfer line into the booster. The beam circulated for up to 400 turns.

5. Installation of the first storage ring components in the ALS building is scheduled for June 1991. Conceptual design reports for all insertion devices have been completed. The permanent magnet blocks needed for the undulators are on hand and undergoing testing. Engineering design of the two insertion device beam lines and a bend-magnet beam line are underway.

Advanced Photon Source
Argonne National Laboratory
Argonne, Illinois

The Advanced Photon Source is designed as a national facility for synchrotron radiation, primarily in the x-ray region of the electromagnetic spectrum. APS is also a third generation synchrotron radiation source. Capitalizing on extensive input from prospective users of the facility, the APS team has designed and is building a source of x-ray beams of unprecedented brilliance. Research at the APS promises to advance knowledge in scientific disciplines that include materials science, medicine, environmental science, atomic physics, biology, earth science,. and chemistry.

Recent accomplishments related to the construction of APS include:

1. The accelerator R&D program is making required contributions to reducing technological risk and assuring optimal design performance at the APS. Accelerator physics studies, both computational and experimental, are addressing beam diagnostics and optimum performance characteristics for the APS accelerators. Development with industry of a computer-controlled vacuum chamber welding technique is nearly complete. Five R&D chamber sections, each ca. 15 ft. long, have been evaluated and base pressures of ca. 4×10^{-11} Torr have been obtained with distributed non-evaporable getter pumping. A second prototype, an 0.8 meter-long storage ring quadrupole magnet, modified to achieve required mechanical stability, has been measured and final design is nearly complete. The linac electron gun has been assembled at ANL and tests will begin, with 60 MeV operation expected by summer 1991. A prototype accelerator rf copper cavity for the storage ring is under test, and will be full-power evaluated up to 250 kW at the test station now being completed.

2. Component R&D is underway on the insertion devices and optical components for APS. Insertion devices are large arrays of permanent magnets that will manipulate the positron beam to produce the x-rays. The intensity of these x-ray beams produces heating of the optical elements that will focus the beams. A 7.5 cm period, 2.4 meter-long APS-designed prototype undulator was fabricated by industry and installed on the U-5 straight section at the NSLS. The data from the undulator run at NSLS supports the design approach and fabrication selected by APS. The ANL-developed liquid gallium method for optics cooling is being refined and will be tested.

3. Nineteen proposals to form APS Collaborative Access Teams, requesting use of 44 beam lines, were received for screening by the APS Proposal Evaluation Board. These proposals represent 432 principal investigators from 18 industries, 77 universities, 7 medical schools, 23 non-federal research institutes, and 9 Federal laboratories. There have been 12 requests for APS standard undulators, 4 each for two types of wigglers, and 4 other devices have been requested. The proposal review process is to be complete by October 15, 1991.

4. Preliminary APS construction activities were approved by DOE in May 1990 and ground-breaking occurred on June 4, 1990. Preparatory site work, including relocation and protection of wetlands, is near completion. On January 24, 1991, the DOE Energy Systems Acquisition Advisory Board approved the next phase of the APS construction. Pouring of the 274 caissons to support the Experimental Hall began on April 25, 1991. Late April 1991 was also the start date for civil-structural construction of the APS Utility Building, the first structure to be erected on the site. In early May 1991 subcontracts were awarded for site utility work and civil-structural construction of the APS Linac/Injection Wing. Subcontracts completed to date are generally below estimate.

Program and Budget Trends

Basic Energy Sciences and its predecessors have funded and conducted basic research programs in the physical and related sciences and managed complex national facilities since the 1940's, contributing to a period of unparalleled scientific growth and achievement. Basic research is a necessary investment in the future. A stable, uninterrupted program is necessary for basic research to thrive, providing the Nation a knowledge base and source of new technology to maintain a healthy economy. Basic Energy Sciences' long-range research complements and undergirds the applied research and development activities of DOE's technology programs. The program's major product is understanding and fundamental knowledge in areas important to DOE.

The new knowledge generated becomes part of the body of information upon which the applied technologies rest. While research to broaden the technology base needed for specific individual energy technology options is extremely important, so also is our need for basic research to build the science base from which totally new technologies will emerge. It is from such basic research that new ideas and concepts will be applied to cause radical improvements in currently identified options or entirely new options.

The following are some recent Basic Energy Sciences Program and Budget Trends:

- *Increased importance to U.S. science of BES' major user facilities as national assets available to industrial as well as academic researchers;*

- *Enhanced efforts to foster communication of scientific results to technologists, for increasing the awareness of BES-supported researchers of scientific issues facing technologists, and the importance of rapid technology transfer to the private sector;*

- *Design, construction and operation of advanced scientific facilities for research of importance to the Nation where the expertise lies primarily at DOE national laboratories, with particular emphasis on forefront research and assurance of environmental, health and safety for such facilities;*

- *Increased emphasis on inter- and multi-disciplinary research activities.*

- *Increased emphasis on science and math education.*

- *Focus on research underpinning the DOE objectives for secure energy and environmental compatibility.*

The budget for FY 1991 is approximately $705.4 million (Table I) of which $36.8 million is for capital equipment and $102.4 million is designated for construction. The budget request to Congress for FY 1992 is $714.7 million.

Two major new facilities are under construction: a light source at LBL in the ultraviolet wavelength regime (1-2 GeV, Advanced Light Source); and a light source at ANL in the x-ray wavelength regime (6-7 GeV, Advanced Photon Source). In addition to these new projects, work continues to maintain and upgrade existing facilities, and to design a new research reactor.

Table 1. Office of Basic Energy Sciences Budget

Operating Expenses (by Subprogram)	Appropriated FY 1991	Congressional FY 1992
Materials Sciences	272.0	257.1
Chemical Sciences	155.6	158.3
Applied Mathematical Sciences	52.1	75.5
Engineering and Geosciences	33.9	35.8
Advanced Energy Projects	24.7	10.8
Energy Biosciences	21.8	24.7
Program Direction	6.1	7.5
Subtotal	566.2	569.7
Capital Equipment	36.8	37.0
Construction	102.4	108.0
Total	705.4	714.7

Table 2 presents a breakdown identifying the major performers who carry out the Basic Energy Sciences program. About 72% of the program is conducted at the national laboratories including Lawrence Berkeley Laboratory and Ames Laboratory, 26% at universities throughout the country, and the remainder elsewhere, including non-profit institutions and industry.

Table 2. Major Performers

Laboratory	**72%**
University	**26%**
Industrial/Other	**2%**

Ames Laboratory and Lawrence Berkeley Laboratory are co-located with universities (Lawrence Berkeley at the University of California, Berkeley, and Ames at Iowa State University) and receive 16% of the BES support going to national laboratories. If they are included with the universities, that portion of the program rises to 42%, with a corresponding decrease under national laboratories. The research supported by BES at Ames and LBL is conducted almost entirely by faculty members and graduate and postdoctoral students.

The funding going to national laboratories includes support for national user facilities. The operation of major scientific facilities continues to require a large commitment of BES funds. Costs for BES' major user facilities are approximately 33% of the operating budget.

The future for BES continues to be more and more challenging as the frontiers of science expand. Current trends are toward greater use of the major facilities, by both DOE and "outside" researchers, and support of new areas of science.

Information Source Summary

More detailed information on the Basic Energy Sciences (BES) subprograms or Major User Facilities is available from the following individuals or reports:

Materials Sciences: Iran L. Thomas, Director, Division of Materials Sciences, ER-13, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-3427. Report available: Materials Sciences Programs Fiscal Year 1990 (DOE/ER-0483P) which summarizes current projects.

Chemical Sciences: Robert S. Marianelli, Director, Division of Chemical Sciences, ER-14, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-5804. Report available: Summaries of FY 1990 Research in the Chemical Sciences (DOE/ER-0144/8), which summarizes current projects.

Applied Mathematical Sciences: David B. Nelson, Director, Scientific Computing Staff, ER-7, Office of Energy Research, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-5800. Report available: Summaries of the FY 1989 Applied Mathematical Sciences Research Program, DOE/ER-0422, September 1989.

Engineering and Geosciences: James S. Coleman, Director, Division of Engineering and Geosciences, ER-15, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-5822. There are two reports available: Summaries of FY 1990 Engineering Research, DOE/ER-0485P; and Summaries of Physical Research in the Geosciences, DOE/ER-0474P, October 1990. Both provide detailed summaries of current projects.

Advanced Energy Projects: Walter Polansky, Acting Director, Division, ER-16, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-5995. Report available: Advanced Energy Projects FY 1991 Research Summaries, DOE/ER-0498T, September 1990.

Energy Biosciences: Robert Rabson, Director, Division of Energy Biosciences, ER-17, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-2873. Report available: Annual Report and Summaries of FY 1990 Activities, DOE/ER-0469P, September 1990.

Small Business Innovation Research: Samuel Barish, SBIR Program Manager, ER-16, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-3054. Reports available: Abstracts of Phase I Awards, 1990, DOE/ER-0472, and Abstracts of Phase II Awards, 1990, DOE/ER-0467. The most recent program solicitation can be obtained by contacting the SBIR Program Manager.

High Flux Beam Reactor (HFBR): David S. Rorer, HFBR - Bldg. 750, Brookhaven National Laboratory, Upton, New York 11973, (516) 282-4056.

High Flux Isotope Reactor (HFIR): Research Reactors Division, ORNL, Oak Ridge, Tennessee 37831, (615) 574-8049.

National Synchrotron Light Source (NSLS): Susan White-DePace, NSLS Department, Building 725B, Brookhaven National Laboratory, Upton, New York 11973, (516) 282-7114.

Stanford Synchrotron Radiation Laboratory (SSRL): K. M. Cantwell, SSRL, Bin 69, P.O. Box 4349, Stanford, California 94305, (415) 854-3300 ext. 3191.

Intense Pulsed Neutron Source (IPNS): T. G. Worlton, Scientific Secretary, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, (312) 972-8755.

Los Alamos Neutron Scattering Center (LANSCE): J. Eckert, MS H805, Group P-8, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, (505) 667-6069.

Combustion Research Facility (CRF): P. Mattern, CRF, Sandia National Laboratory, Livermore, California 94550, (415) 422-2520.

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