Basic Energy Sciences, one of several major program offices in the Department of Energy's Office of Energy Research, continues to play an important role in the support of basic research in the United States. The program is strongly oriented toward developing the information and understanding needed to maintain and strengthen U.S. long-term technological capability.

This program is organized mainly along the lines of the scientific disciplines to facilitate interaction with the research community. Often, however, the basic research conducted under the auspices of several of the divisions has a common underlying theme; for example, Chemical Sciences and Energy Biosciences intersect in the important areas of photochemistry, photosynthesis, and plant science while Materials Sciences, Chemical Sciences, and even Energy Biosciences all deal with aspects of catalysis. A survey of research activities relevant to improving our insight into long-term problems and solutions of a particular technology will usually span several disciplines. Conversely, a given project can impact more than one energy technology.

This report is a summary document on the Basic Energy Sciences program, its overall scope, the kinds of activities carried out, and the unique facilities that have become so important to our ability to conduct forefront research.

Donald K. Stevens
Associate Director for
Basic Energy Sciences
Office of Basic Energy Sciences 1986 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. 20545

Published by
U.S. DEPARTMENT OF ENERGY
Office of Scientific and Technical Information
The United States has evolved a tradition of leadership in science and technology that has led other nations to emulate us. Today our basic research activities, carried out mainly in universities and government laboratories, underpin continuing U. S. leadership in science, train our future scientists, and contribute to our social and economic well-being. Attainment of our national goals—energy self-sufficiency, improved health and quality of life for all, economic growth, national security—depends directly or indirectly on basic research. Knowledge and discoveries resulting from research provide the stimulus for technology development and economic growth.

The most prestigious of our accomplishments in 1986 was the recognition accorded by the Nobel Prize committee to Yuan T. Lee, University of California; Dudley R. Herschbach, Harvard University; and John C. Polanyi, University of Toronto, for their experimental and theoretical research on the chemistry of colliding molecular beams. Lee and Herschbach's research work had been carried out at DOE's Lawrence Berkeley Laboratory (LBL) with support from the Atomic Energy Commission, predecessor to DOE. The reactions of colliding beams of atoms and molecules were first observed by Sheldon Datz at DOE's Oak Ridge National Laboratory in the mid-1950s. It was at LBL, however, where these observations were followed up. The research activities leading to the 1986 Nobel Prize in chemistry were described in an article in the LBL Currents in October 1986. The article is included as a special "Nobel Prize Chemistry Award" feature in the next section.

Less spectacular than a Nobel Prize, but significant nevertheless, was the development this past year of a new technique to control alloy structure at the microscopic level during the synthesis of a magnetostrictive alloy. "Magnetostriiction" is a change in shape or volume of a material subjected to a magnetic field, a property that can be used in many practical applications. Practical application has been precluded however because, until recently, this property could be produced only in small, discrete volumes or "regions" within bulk material; because these microscopic magnetostrictive "regions" are randomly oriented, on a larger scale the useful magnetostrictive property is effectively cancelled out. At Ames Laboratory, a new synthesis technique has been developed to prepare the magnetostrictive alloy, Terfenol-D, that overcomes this problem and allows bulk quantities to display magnetostrictive properties. Terfenol-D is an alloy of iron containing the rare-earth elements terbium and dysprosium. A crystal of this alloy and an apparatus used for its preparation are shown in the photograph. Two different techniques have been successfully used to produce single crystals of Terfenol-D. The processing technique is automated and is highly reproducible.

Currently the Ames Laboratory at Iowa State University is the only source for Terfenol-D, which it supplies to research and prototype development programs. The projected commercial demand is approximately 2000 kg/yr (up 40 times from the present R&D demand). The Ames Laboratory is working with industry to develop and transfer the technology for mass production. Commercial applications for rare-earth–iron magnetostrictive materials are underground devices for oil exploration, micropositioners for laser mirror actuators, fuel injection systems for diesel engines, robot components such as hands, wrists, elbows, etc., and underwater sonar devices for naval defense systems.

In another area, a novel composite material permitting photosynthesis and catalysis reactions to be linked together was prepared this past year at Oak Ridge National Laboratory. Photosynthesis takes place in the chloroplasts of green plants. A chloroplast is made up of organic molecules that work together using light from the sun to produce carbohydrates from carbon dioxide and water. The particular molecule in the chloroplast that traps light is chlorophyll, while other complex molecules participate in carrying out the sequence of reactions that eventually produce carbohydrates.

The reactions that occur during photosynthesis depend on electron transport at the molecular level. By coating the chloroplast with platinum, electrical contact is made with the photosynthetic electron transport chain. This contact effectively shunts electrons away from the normal electron transport chain to the platinum which then catalyzes the formation of hydrogen and oxygen from the available chemical reactants. This new composite material, a "platinized chloroplast," thus allows a solar energy driven system to produce hydrogen and oxygen, a novel approach using green plant biotechnology for energy
production from renewable resources.

The following pages describe the program of the Department of Energy's Office of Basic Energy Sciences, which is responsible for basic research in the scientific disciplines likely to contribute to our long-term energy goals. The Basic Energy Sciences subprograms and facilities are discussed, along with an abbreviated budget summary and an outline of plans for the future. Reports referenced are normally available from the National Technical Information Service, U. S. Department of Commerce, Springfield, VA 22161.
Yuan T. Lee wins Nobel Prize

By Lynn Yarris

Yuan T. Lee has become LBL's ninth Nobel laureate. A chemist with the Materials and Molecular Research Division, and professor at UC Berkeley, Lee has won the 1986 Nobel Prize in chemistry for his work with crossed molecular beams.

Sharing the prize with Lee are Dudley Herschbach of Harvard University and John Polanyi of the University of Toronto. Herschbach was a chemist with LBL in 1960 when he led one of the first successful crossed molecular beam experiments — a crossing of potassium and methyl iodide beams. Lee was one of his graduate students then.

Of the three Nobel Prize winners, the Royal Swedish Academy of Scientists said: "Their research has been of great importance for developing a new field of research chemistry — reaction dynamics — and has provided a much more detailed understanding of how chemical reactions take place."

In winning science's most prestigious honor, Lee joins such other LBL luminaries as Ernest O. Lawrence, Glenn Seaborg, Edwin McMillan, Owen Chamberlain, Emilio Segre, Donald Glaser, Melvin Calvin, and Luis Alvarez.

"Yuan Lee is a world leader in the field of chemical reaction dynamics," said LBL Director David Shirley. "His work has advanced crossed molecular beam science beyond alkali metals to include all chemical systems, and has played an important role in understanding the dynamics of chemical reactions on an atomic scale."

It has been quite a year for Lee. In March, he received the National Medal of Science, this country's highest science award. The 1986 Peter Debye Award from the American Chemical Society also went to Lee. These awards join a raft of other recognitions, including the 1981 E. O. Lawrence Award.

"I thought they were congratulating me for giving a good lecture," said Yuan T. Lee, telling reporters how he first learned about winning the 1986 Nobel Prize in chemistry. Lee, who was attending a meeting in Los Alamos when the award was announced, was told about his victory while riding in an elevator.

A native of Taiwan, Lee, 49, earned his B.S. at the National Tsinghua University, before coming to Berkeley, where he received his Ph.D. in chemistry in 1965. He became involved with crossed molecular beam research while working as a grad student with Dudley Herschbach, with whom he shares the Nobel Prize (along with John Polanyi), and whom he calls "my mentor."

Lee followed Herschbach to Harvard University to do postdoc work until 1967. After seven years at the University of Chicago, he returned to Berkeley, where he now holds a dual appointment in MMRD and a professor in UC Berkeley's chemistry department.

All employees are invited to attend a reception in honor of

Nobel Laureate Yuan T. Lee

from 3 to 5 p.m. today in the LBL Cafeteria.
The 1986 Nobel Prize in chemistry was awarded to two American and one Canadian chemist for developing both the theories and the experimental instruments that allow chemists to discover what happens at the atomic level when a chemical reaction takes place. The two Americans are Yuan T. Lee and Dudley R. Herschbach; the Canadian scientist is John C. Polanyi. Lee’s work, supported by the group in the Atomic Energy Commission that later became Basic Energy Sciences, is presented in the article on page 4 reprinted from Lawrence Berkeley Laboratory’s Currents of October 17, 1986.
Basic research requires long-term commitments of resources and people with little promise of early success or return on investment. The support of long-range basic research has emerged as the particular responsibility of the federal government. Within the Department of Energy, the mission of the Office of Energy Research is to support advanced research directed toward providing insight into fundamental science and associated phenomena. The Office of Basic Energy Sciences (BES) is responsible for long-range basic energy-related research. Its goal is to provide the scientific underpinning needed to give us viable energy options in the future.

BES is organized primarily along scientific discipline lines as shown in Figure 1.* This structure helps the research community identify programs of interest to them, but it does not prevent interdivisional support activities in areas of mutual interest. Examples of interdivisional activities are catalysis and surface science involving both Materials and Chemistry, photosynthesis involving both Chemistry and Energy Biosciences, and mechanical fracture involving both Materials and Engineering.

BES supports about 1200 individual research projects, each selected because of (1) its relevance to our long-range energy research goals, (2) its role in a responsive national research program, and (3) its scientific merit.

The knowledge that results from BES-sponsored research becomes an integral part of the body of information on which the applied technologies rest.

Research to broaden the technology base needed for identified energy options is extremely important. Even more important, however, is the need for continuing basic research, unconstrained by preconceived notions of what technologies will be important several decades from now, so that new, as yet unidentified, options may emerge. Thus a comprehensive program of basic energy-related research is essential to fulfilling DOE's energy supply mission.

The Office of Basic Energy Sciences plans and administers DOE's programs of basic energy research in the physical, biological, and engineering sciences.** Key aspects of the BES program are:

- Orientation toward DOE's energy mission
- A principal role in the physical and engineering sciences efforts of the nation
- Major support of university research and research at the national laboratories
- Construction and operation of large and complex scientific facilities
- The multipurpose national laboratories are national assets and play an essential role in U.S. science and technology by maintaining expert scientific and engineering staffs, building and operating complex scientific facilities, and undertaking large interdisciplinary projects. 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 player in the newly evolving national goal of enhancing our economic competitiveness with other nations through increased and more rapid use of our scientific results for technology applications.

Many areas of modern science require large and costly facilities to develop information not otherwise attainable. The large, expensive, unique facilities in the BES program are made available for use by the entire scientific community to the extent that funds permit. The operation of major scientific facilities continues to require 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 Los Alamos Neutron Scattering Center, and high-voltage and atomic resolution microscopes.

Most of the scientists involved in BES research programs are located at universities and

---

*Mathematical Sciences activities, while budgeted under BES, are administered by the Scientific Computing Staff which reports directly to the Director of Energy Research.

**High Energy and Nuclear Physics and the Health and Environmental Sciences research are carried out by other offices in Energy Research.
national laboratories. In addition, access to qualified scientists not directly supported by BES is provided at the major user facilities. Although about 30% of BES funding directly supports university-based research, indirect support 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 Basic Energy Sciences program also participates in the congressionally mandated Small Business Innovation Research program, which was initiated in FY 1983. A number of BES projects are being supported at highly specialized, research-oriented small business firms. The level of this effort was 1.25% of the BES operating expenses in FY 1986, i.e., about $4,200,000.

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, and the U. S. Geological Survey have working groups and committees that routinely exchange information and coordinate program activities in areas of common interest such as nuclear data, chemistry, geophysics, materials, and combustion 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 problem areas in their

Fig. 1 Organizational chart of the Office of Basic Energy Sciences.
work. Finally, study results normally are published in the open literature to make them available to the scientific community at-large.

Current trends are toward greater use of the major facilities, by both DOE and "outside" researchers, and strengthening of research in the following areas of science:

- **Surfaces**: their modification, interfaces, reactions at surfaces
- **Solids**: their properties and structure including grain boundaries, electronic and magnetic properties, condensed matter theory, atomic transport, amorphous materials, and structural ceramics
- **Plants**: including genetics, response to stress, and photochemistry
- **Geothermal energy resources**: their occurrence, characterization, and chemical and thermal properties
- **Multiphase systems**: their transport properties and their chemical and physical behavior

During the decade from 1975 to 1985, BES experienced a significant expansion in its responsibilities to include basic research relevant to nonnuclear energy technologies. More recently, there has been an increased emphasis on assisting U.S. industry in the development of what has come to be known as "Technology Transfer," operated through the national laboratories as a means of enhancing the flow of research results to the private sector.

The future for BES continues to be more and more challenging as the frontiers of science expand. Experiments at the cutting edge of science involve extremes: extremely short reaction times, vanishingly small concentrations, species with only fleeting lifetimes, and measurements under extreme conditions of temperature and pressure. Carrying out such experiments requires increasingly more complex instrumentation. Examples of BES's efforts to meet such challenges include the development of advanced synchrotron radiation facilities, advanced neutron sources to increase our understanding of the structure of materials, and the establishment of electron microscopy centers.

As noted earlier (Fig. 1), BES is organized along scientific discipline lines. Research is managed under six divisions: Materials Sciences, Chemical Sciences, Engineering and Geosciences, Advanced Energy Projects, Energy Biosciences, and Carbon Dioxide Research. The activities under each of these divisions and under the Scientific Computing Staff are described briefly in the "Subprograms" section.
Tailoring Surfaces by Ion Implantation: The Evolution of a New Technology

The establishment of ion implantation as a viable industrial technology is an excellent example of how a field of technology develops from many scientific contributions over an extended period of time. The Department of Energy and its predecessor agencies contributed heavily to the evolution of this important modern technology.

The ion sources developed for electromagnetic separation of uranium isotopes as part of the Manhattan Project in the early 1940s formed the basis for present-day ion implantation equipment and techniques. Later work performed under Atomic Energy Commission (AEC) and DOE/BES sponsorship made major contributions to the fundamental understanding of ion implantation and to equipment development.

**What is Ion Implantation?**

Ion implantation is a technique for incorporating virtually any element into the near-surface region—the surface layers—of a solid. Atoms of the element to be implanted are ionized—electrically charged—and the ions are extracted and accelerated to form a high-energy ion beam directed at the surface of a solid target. Ions striking the target penetrate it; the depth of ion penetration into the solid can be precisely determined by controlling the energy of the ion beam. Using this technique, combinations of atoms that cannot be mixed as solids or liquids have been alloyed, and materials have been mixed at higher concentrations than were ever before possible. In addition, completely new lattice structures and metastable phases have been produced. Ion implantation also provides unprecedented freedom and control in tailoring surfaces to have properties that are independent of the bulk properties. Specific applications include tailoring the electrical properties of semiconductors; fabrication of superconducting surface alloys; inhibition of friction, wear, and corrosion of metals; increasing the hardness of ceramics; and fabrication of a variety of new or metastable surface alloys, compounds, and extended solid solutions.

**Semiconductor Technology**

The first important technological application of ion implantation was in semiconductor technology. Ion implantation of semiconductors became an identifiable discipline in the early 1960s, as AEC-sponsored research from the seemingly disparate areas of isotope separation, atomic and nuclear physics, and nuclear chemistry converged with semiconductor device research being pursued in the private sector. Many research laboratories played important roles in the early developments including Sandia National Laboratories, supported by AEC's Division of Military Applications, and Oak Ridge National Laboratory (ORNL), supported by BES and its predecessors. Ion implantation has since become an essential processing step in the fabrication of integrated circuits for the microelectronics industry. Without ion implantation our computer and communications industries would not exist as we know them today.

BES has continued supporting basic research on semiconductor materials. This research has been coupled with research making use of laser annealing technology, an outgrowth of laser research. By combining these two processing techniques, it is now possible to fabricate semiconductor alloys that are essentially a new class of materials that have unique lattice structures in their ion-implanted surface regions. Through the use of extremely intense, short (one billionth second) bursts of laser light, ion-implanted semiconductors can be melted and recrystallized so that the implanted, or dopant, atoms are incorporated into particular lattice sites that are electrically active. The concentrations of implanted atoms at these lattice sites can be 1000 times greater than could be attained with conventional processing techniques. This procedure has been used at ORNL in a program to fabricate a variety of semiconductor structures including solar cells with efficiencies as high as 19.5%.

**Improvement of Surface Physical and Chemical Properties**

BES-funded research in ion implantation also has had a major impact in technologies for tailoring the physical and chemical properties of metal and properties of metal and insulator surfaces. The initial purpose for this research was to carry out fundamental studies of the physical and chemical properties of materials not normally available. With ion implantation, any mixture and relative proportion of elements could be obtained, including those that would not mix at all in the molten state. Subsequently, it was observed that tailored surface could be produced by ion implantation without altering the proper-
ties of the bulk materials. In some applications, beneficial properties also are derived from the microstructural damage that results from the passage of the ions through the material.

Deposited films, for example, can often be made more adherent by the ion-induced damage found at the interface of the film with the substrate. A promising surface tailoring result stemming from BES-sponsored research is an ion implantation process that reduces the wear rate of steel. When stainless steel is treated with carbon and titanium ions to produce a surface alloy containing about 20% of each element, the surface region of the steel loses its crystalline order and transforms to an amorphous, or glassy, state. This treatment decreases the metal's coefficient of friction and slows its wear rate. In studies at Sandia National Laboratory, the coefficient of friction for stainless steel treated in this manner was reduced from 0.7 to 0.2. The wear rate, even for the high strength steels used for bearings, can be reduced to one-tenth of the value for nontreated high strength steel.

Currently, BES is exploring the effects of implanted ions on the surface properties of high-temperature ceramic materials. Experiments performed at the Surface Modification and Characterization Facility at Oak Ridge National Laboratory have demonstrated that the hardness and fracture toughness of alumina are increased by nearly 50% by implanting selected dopants. These improvements were found to persist to temperatures as high as 1500°C for some dopant species, making ion implantation an attractive candidate for surface modification of ceramic bearing materials for high temperature applications. Ion implantation at low temperatures or with large concentrations of ions renders the ceramic surfaces amorphous and causes surface hardness to decrease while maintaining improved fracture toughness. Similar results have been obtained with other ceramics including silicon carbide, silicon nitride, titanium diboride, and zirconia.

Although the above-mentioned phenomena were only recently discovered, implantation and related treatments for improving surface mechanical properties are attracting attention for potential defense and commercial applications. Defense applications under investigation are those in which friction and wear must be controlled in mechanical parts that function for long times in extreme environments where lubricants break down or evaporate, e.g., in long-lived satellites. Commercial interest focuses on ion treatment for critical components such as bearings in jet engines and gyroscopes and for precision tools for industrial processes in which the cost of the part, or the cost of stopping production to replace the part, makes longevity crucial. For example, Spire Corporation has applied the carbon/titanium ion implantation procedure to produce refrigeration pistons that can operate without lubrication in low temperature pumps and to produce low friction ball bearings that operate without lubrication in vacuum.

**Corrosion Inhibition**

In addition to the control of mechanical surface properties, chemical changes from the implantation of the proper atomic element can provide remarkable improvements in the corrosion behavior of the treated material. One application of this effect is the treatment of titanium alloy knee and hip joint prosthetic devices. Longevity of such medical implants in the human body is crucial. However, in the environment of body fluids, corrosive wear produced by the motion of a metal joint in its polyethylene socket can severely degrade the joint. Researchers at Oak Ridge National Laboratory have shown that implantation of titanium with nitrogen ions can slow the metal wear rate by factors of up to 1000. This remarkable improvement means that an implanted hip joint would never have to be replaced because of corrosive wear. This technology is now in the private sector with hundreds of ion-implanted replacement joints (photo on opposite page) being produced each year and used in human subjects. The cost of this treatment is modest, representing only 1% of the total cost of a joint replacement. Johnson and Johnson is the major distributor of ion-implanted surgical replacement joints.

The promise shown by results from research in ion implantation metallurgy has led many non-DOE and industrial researchers into this area of investigation. For example, it has been shown by Bell Laboratories that implanting a few platinum ions—less than 20 millionths of a gram per square centimeter—can give a thousandfold improvement in the corrosion resistance of steels. Although platinum is a precious metal, the treated layer is so thin that the cost of the implanted platinum is only a few hundredths of a cent.
per square centimeter. Similar improvements have been found for implanting platinum into titanium to reduce electrochemical corrosion. Again, small amounts of platinum implanted into the surface give protection equivalent to expensive titanium-platinum alloys.

**Radiation Effects Studies**

During ion implantation, lattice defects are created from collisions between the target atoms and the implanted ions. Thus, ion implantation can be used for fundamental studies of these defects and associated materials properties. For example, for many years ion beams have served to simulate the neutron bombardment resulting from fusion and fission nuclear reactions. Neutron bombardment causes some metals to increase in volume, or swell, by several percent. This swelling can interfere with the close mechanical tolerances required in reactor design. BES-funded research helped to demonstrate that ion implantation could be used to simulate this damage, to investigate the basic mechanisms of radiation damage, and to aid in the search for materials resistant to swelling. Because ion implantation can produce the same amount of damage much more quickly than neutrons, it has facilitated the understanding and characterization of this materials problem.

During the BES studies of radiation effects, the important phenomenon of radiation-induced segregation was discovered. In the early 1970s, researchers at Argonne National Laboratory demonstrated that ion bombardment can cause large changes in the chemical composition near commonly occurring lattice imperfections. Subsequent studies of this phenomenon led to the discovery of effects that are induced by the segregation processes themselves and that adversely affect the swelling resistance of alloys. Because of the technological significance to reactors, many aspects of the basic findings derived from this research have been incorporated into fission and
fusion reactor alloy development programs.

The impact of these radiation effects studies now extend well beyond reactor applications. By contributing to a fundamental understanding of ion implantation, this research has led to a convergence of the more traditional field of radiation effects and the newer area of ion beam surface modification. For example, studies at Argonne have shown that in addition to the implanted ions, the processes of radiation-enhanced diffusion and radiation-induced segregation contribute to changes in the near-surface composition of an alloy during ion implantation. These processes are of particular significance because they can alter the composition to depths which are much greater than the implanted ion range. By altering various parameters such as irradiation temperature, ion mass, ion energy and current density, and initial alloying distribution, radiation-enhanced diffusion and segregation processes can be exploited to produce a rich variety of the near-surface composition profiles.

Emerging Technologies

While conventional ion implantation techniques are widely accepted and used by industry, the search for improved techniques and for enhanced understanding of the mechanisms behind the techniques continues. For example, researchers funded by BES and other sources are finding that a variant of ion implantation known as ion beam mixing offers promise for supplying thicker alloyed layers and more adherent thin film coatings less expensively, thus further extending the applicability of ion-related treatments. In ion beam mixing, a film of material is vapor or sputter deposited onto the surface to be treated and, subsequently or simultaneously, the surface is exposed to a beam of ions. Collisions produced by these energetic ions intermix the atoms of the deposited film with those of the host material. Because this process requires implantation of fewer ions, it is more economical than conventional ion implantation.

Ion implantation also has potential applications in the important area of silicon-on-insulator (SOI) technology. Complex microcircuits and memories formed as SOI sandwiches are displaying much higher speeds and greater reliability than conventional silicon technology and are expected to contribute significantly to the next generation of ultrahigh density integrated circuits. There is also military interest in SOI circuits because of their intrinsic insensitivity to radiation. Although ion implantation is not yet used in the fabrication of the current generation of devices, this technique is being actively pursued by most major semiconductor firms for the next generation of high density memories and for three-dimensional integrated circuits. Several high capacity oxygen and nitrogen ion implanters have been sold to companies performing high density circuit development. These circuits are intrinsically insensitive to radiation damage and thus are also of military interest.

A recently funded BES initiative called ion beam deposition offers a new approach to the fabrication of isotopic thin films and heterostructures. By decelerating ions from an ion implantation accelerator to very low energies, isotopically pure films of virtually any element can be deposited on any substrate. This technique has been utilized to produce surface films of silicon and germanium at temperatures as low as 375°C and isotopic thin films and heterostructures of both semiconductors and metals. Although primarily a research tool, the fundamental understanding of thin film processing derived from this technique may lead to major advances in low temperature fabrication—a promising new technology for future semiconductor devices.
Subprograms

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

Materials Science

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 and why they are that way; how its properties relate to its structure; and what phenomena are involved in, and govern, its behavior. This understanding is essential to the development of future energy technologies. It is well known that materials problems and limitations often restrict the performance of current energy systems and the development of future systems. Some needs to which Materials Sciences research ultimately contribute include:

- Developing new or substitute materials
- Tailoring materials to satisfy defined requirements
- Predicting materials problems and service life
- Improving the ability to successfully attack unforeseen materials problems in advanced energy systems
- Improving the theoretical and experimental capability to analyze the fundamental structure and properties of materials

With support at an operating level of $132,600,000 in FY 1986, Materials Sciences provided more than one-third of the total federal funding for basic materials research.

Materials Sciences places emphasis on selected generic areas of fundamental importance and on areas where problems are known to exist or are anticipated. Some research is related to a single energy technology (e.g., photovoltaic materials for solar energy conversion); some research has applicability to many technologies.
simultaneously (e.g., embrittlement of structural materials in the presence of hydrogen); and still other research has more fundamental implications underpinning all materials research (e.g., mechanisms of atomic transport in solids and computer modeling of materials phenomena). The research is conducted in a variety of institutions—DOE laboratories, universities, and, to a lesser extent, industrial installations—and uses the talents of metallurgists, ceramists, solid-state and condensed-matter physicists, and materials chemists.

In addition to maintaining an appropriate mix of long-term scientific multitechnology, and single-energy-technology-related research, some balance must be retained among forefront, large, facility-related research and small individual projects. Materials Sciences has supported the construction and use of major facilities in the pursuit of its research goals, including the National Synchrotron Light Source (NSLS) and the High Flux Beam Reactor (HFBR), both at Brookhaven National Laboratory; the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory; the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory; the Los Alamos Neutron Scattering Center; the electron microscopy facilities at Oak Ridge, Argonne, and Lawrence Berkeley Laboratories and at the University of Illinois; and the Stanford Synchrotron Radiation Laboratory.

The operation of these facilities required about 21% of the FY 1986 operating budget of the Materials Sciences subprogram, not including the research associated with them. Most of these facilities are unique, as is the research carried out at these sites, and they are available to qualified users outside the DOE laboratory complex.

The Materials Sciences subprogram is the basic research program in DOE which underpins materials development efforts in the energy technologies. 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 workshops and reports of the Materials Sciences Division’s Council on Materials Science (a body with representatives from academia, industry, and DOE laboratories) help to focus attention on critical issues. In 1984, panel studies on Novel Methods of Materials Synthesis and on Theory and Computer Simulation of Materials Structures and Imperfections were held. In 1985, the two studies were on Micromechanisms of Fracture and Bonding and Adhesion at Interfaces. The Department’s and other applied materials research workers interact and exchange information through a number of mechanisms, including a formalized Research Assistance Task Force. An example of a recent task force is one held with DOE’s Fossil Energy Office and the Electric Power Research Institute entitled Research Avenues for Controlled Growth of Corrosion Resistant Scales in Advanced Coal Conversion Systems.

Current emphases and trends include greater use of the major facilities, use of supercomputers in calculations and modeling of materials phenomena, high strength and high conductivity polymers research, surfaces and interfaces research, and materials synthesis and processing science.

More detailed information on the activities of the Materials Sciences Division can be obtained from I. L. Thomas, Director, Division of Materials Sciences, Office of Basic Energy Sciences, Department of Energy, Washington DC 20545, (301)353-3427. A detailed summary of current projects is published annually. The most recent (September 1986) is entitled Materials Sciences Program, Fiscal Year 1986 (DOE/ER-0295).
The Chemical Sciences subprogram sponsors experimental and theoretical basic 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 Chemical Sciences subprogram objective is to expand our knowledge in the various areas of chemistry; the long-term goal is new or improved processes for developing and using domestic energy resources. At a budget level of $104,300,000 in FY1986, this subprogram is a major source of federal support for basic chemical research in the United States.

Chemical phenomena and processes apt to be important to energy technologies are emphasized in formulating the program. Research in some areas, such as chemical catalysis where learning 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.

The Chemical Sciences subprogram includes research that impacts fields such as photovoltaics (the conversion of solar energy to electricity), production of fuels and chemicals from coal, catalysis, nuclear waste separation, conversion of biomass (wood, leafy materials) into liquid fuels using...
enzymes or microorganisms, separation of metals from low-grade mineral resources, combustion, and detection and measurement of harmful by-products of energy processes. Equally important is the fundamental research into chemical processes and phenomena which have no immediately identifiable related energy technology. A typical example of such an effort is the study of molecules, atoms, or ions that have been impacted by laser beams, have energy levels above normal and thus chemical behavior also different from what normally occurs. Disciplinary areas covered by Chemical Sciences work include physical, organic, and inorganic chemistry; chemical physics, atomic physics; photochemistry; radiation chemistry; thermodynamics; thermophysics; and analytical chemistry.

One of the areas in which considerable progress has been achieved over the past several decades has been the elucidation of the very complex chemistry of photosynthesis. Various research approaches have led to an improved understanding of the structures of the molecules and of the chemical reactions involved. Most recently, a “photoreaction center” was synthesized in the laboratory modeling an important aspect of the photosynthetic process. A photoreaction center is a molecule or a group of molecules that absorb light energy which causes an electron to move from one end of the reaction center to another. This “charge separation” initiates the chemical reactions of photosynthesis and is a critical step in triggering the photosynthetic process. In the natural photoreaction center, light is absorbed by chlorophyll followed by rapid electrical charge separation involving other components in the photoreaction center. A key feature of nature’s system is that the charge separation takes place in several successive steps. By learning how to control the length of time (still exceedingly brief) that the charges are kept apart before they recombine, a whole area of using photosynthetic-like processes to carry out useful chemical reactions may be opened up.

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 National Synchrotron Light Source, which is able to provide high intensity X-ray and ultraviolet radiation for inducing specific chemical reactions and for probing structure 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. DOE laboratories also encourage interactions between basic researchers and research and development teams working in energy technology areas.

Universities perform about a third of the Chemical Sciences supported research. National laboratory scientists, who perform most of the research supported by Chemical Sciences, also interact with research workers in the private sector, such as the automotive and petroleum industries. Only a small portion of the Chemical Sciences program of research is conducted in industry.

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 Conference, 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 the National Academy of Sciences/National Research Council report on Opportunities in Chemistry and the Energy Research Advisory Board review of the report (Review of the National Research Council Report: Opportunities in Chemistry) 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.

**Heavy Element Research**

The nuclear energy programs of DOE need a broad-based knowledge of the chemical and physical behavior of the actinide elements (atomic numbers 90 through 103) as well as specific information and data on their behavior in fuel reprocessing streams, in nuclear waste host materials, and in the environment. Heavy element chemistry research helps meet these needs. Ongoing studies of the actinide elements include their behavior in aqueous and non-aqueous solutions, photochemistry, chemical reactivity, spectroscopy, and chemical physics.

The study of actinide chemistry is largely limited to the national
laboratories because high levels of radioactivity are involved, but some tracer work is done at universities. The national laboratory facilities provide opportunities for visiting scientists from foreign and domestic universities and other institutions to collaborate with U. S. investigators. The research materials used in these studies are produced by the neutron irradiation of curium (atomic number 96) targets in the High Flux Isotope Reactor (HFIR). These targets are processed in the Transuranium Processing Plant (TPP) to extract and purify the other higher atomic number actinides produced. Actinide research samples are allocated to investigators engaged in DOE research programs by the Research Materials/Transplutonium Program Committee. This Committee coordinates the production of these research materials with the needs of the investigators, advises DOE on the allocation of the materials, and approves proposals for the use of these materials in international collaborations.

**Isotopes Separations**

In addition to its research and information-gathering activities, Chemical Sciences also supports the electromagnetic separation of stable isotopes for a sales program and for a Research Materials Collection of samples for use in non-destructive research of interest to the DOE. The stable isotopes and the rare, heavy radioactive isotopes are made available by sales and loan for use in research, medicine, and industry. These efforts constitute the western world's only source of isotopic research samples in significant quantities, and these materials are sold or loaned to institutions throughout the world. The separation of stable isotopes is accomplished at the Oak Ridge National Laboratory (ORNL) and is managed by ORNL and the DOE through the Oak Ridge Operations Office. Because of the importance of this service to a worldwide community, an outside advisory committee and a user's group provide recommendations to ORNL on the isotope needs and priorities of the user community. For additional information on stable isotopes separations see the section on Calutrons.

Additional information on the Chemical Sciences subprogram can be obtained from Robert S. Marianelli, Director, Division of Chemical Sciences, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545, (301)353-5804. A detailed summary of current projects is published annually. The most recent (September, 1986) is entitled *Summaries of FY 1986 Research in the Chemical Sciences* (DOE/ER-0144/4).

---

**Applied Mathematical Sciences**

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

The advancement of science traditionally has depended on experiments for data and on theory for understanding. Today there exists a third and equally important ingredient in scientific research: computational science. Computational science is a hybrid between theory and experiment. In some cases computations provide insights into experimental data; in others, computations simulate the ideal experiment for testing an analytical model. The emergence of computational science as an important element in scientific research and technology development results from our increased ability to do computational modeling of complex physical problems and from the enormous power of the modern supercomputer. This combination allows scientists and engineers to model complex problems in a realistic way and to obtain more accurate answers than were possible just 5 years ago.

The objectives of the AMS subprogram are to meet both the immediate needs for supercomputer access by the research programs supported by the Department's Office of Energy Research, not including the Office of Fusion Energy, and the long-range computational research needs of the Department.

**Mathematical Sciences Research**

The primary objective of the Mathematical Sciences Research activity is to advance our understanding of the fundamental con-
cepts of mathematics, statistics, and computer science that underly implementation of prototypes of several potentially strong candidate architectures; this facet will be an important proof of concept activity.

University researchers play the major role in generating ideas and research software, in training graduate students, and in generating new applications. National laboratory staff are in the forefront of tackling real world, large-scale scientific problems and have unique resources for participating in these research projects. Industry likewise has a unique role in providing state of the art production and testing facilities.

Industry also stands to reap great benefits in the understanding of future architecture and software issues that currently tend to limit industry use of supercomputers. These cooperative projects should make the transfer of technology from the academic and laboratory research environment to industry as rapid as possible. The DOE program will be coordinated with programs of other agencies in order to share common facilities wherever possible.

**Energy Sciences Advanced Computation**

The Energy Sciences Advanced Computation activity provides scientific supercomputer access required by researchers in the Energy Research programs except for Fusion Energy. While DOE has been a leader in the use of supercomputers in its Defense and Magnetic Fusion programs, several research programs have not had access to modern larger computers. In FY 1985, the use of the National Magnetic Fusion Energy Computational Center (NMFECC) network was expanded to researchers supported by the following DOE programs: High Energy and Nuclear Physics, Basic Energy Sciences, and Health and Environmental Research. A Cray-XMP/22 was recently added to the computer capacity at the NMFECC center at Livermore, and expansion of the communications network began. In addition, a new supercomputer research institute at Florida State University was initiated at the direction of Congress, and a Cyber 205 supercomputer was installed and linked to the MFE network in early 1985 for use by Energy Research supported scientists. A description of this activity may be found in *The Role of Supercomputers in Energy Research Programs*, (DOE/ER-0218), February 1985.

Additional information on the Applied Mathematical Sciences subprogram can be obtained from David B. Nelson, Director of Scientific Computing Staff, ER-7, Department of Energy, Washington, DC 20545, (301)353-5800. A detailed summary of current projects is published periodically. The most recent (November 1986) is entitled *Summaries of the FY1988 Applied Mathematical Sciences Research Program* (DOE/ER-0306).
Engineering and Geosciences

The Engineering and Geosciences subprogram conducts fundamental research for DOE in two fields: Engineering and Geosciences. 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 Energy Research Advisory Board, panels of the National Academy of Sciences, specially convened workshops, and individual interactions with scientists and engineers from universities, federal laboratories, industry, and related federal programs.

Engineering Research

The Engineering Research objectives are (1) to improve and advance our knowledge of processes underlying current engineering practice, and (2) to expand the technical data base and knowledge of fundamental concepts for solving anticipated and unforeseen engineering problems in energy technologies. Fundamental research is supported in both traditional engineering disciplines and interdisciplinary areas, addressing problems related to energy conversion, distribution, and utilization. At present three research areas are receiving high priority:

- Mechanical Sciences, including fluid mechanics, heat transfer, and structures
- Systems Sciences, including system analysis and control, and instrumentation
- Engineering Analysis, including engineering data collection and compilation, nonlinear systems, and nonequilibrium systems

While the fundamental engineering research is aimed at long-term goals, often important applications emerge surprisingly early. For example, recent studies of methods for measuring some properties of low-energy electrons have led to possible very sensitive, but nonintrusive, means of detecting concealed explosives.

Under Engineering Research, the Center for Engineering Systems Advanced Research (CESAR) was established in 1983 at the Oak Ridge National Laboratory to address fundamental issues in intelligent machine technologies. An experience base at ORNL already existed in the form of remote and tele-operation applications for handling radioactive materials. The CESAR program is building on that experience in performing research on intelligent machines, i.e., manmade systems capable of autonomous decision making and action. Such intelligent machines are to govern themselves in accomplishing given objectives, managing their own resources and maintaining their integrity with only loose human supervision. The test bed for current research results is HERMIES-II, a low cost system incorporating such capabilities as mobility, manipulation, and sensory feedback—features useful for validating various concepts. This system is controlled by a novel parallel processor.

A joint research venture, under Engineering Research auspices, also was undertaken between the Idaho National Engineering Laboratory and the Massachusetts Institute of Technology to address, in a cooperative and supportive fashion, research in the areas of plasma process engineering, automated welding, fracture mechanics, and engineering analysis and design methodology. A steering committee, with representation from universities, private industry, and national laboratories has been established to provide guidance for this four-part research program. Personnel exchanges, including graduate students, have been a feature of this collaboration.

Geosciences

The objective of the Geosciences activity is to develop a quantitative, predictive understanding of the energy-related aspects of geological, geophysical, and geochemical processes both in the earth and at the solar-terrestrial interface.

Discipline-oriented areas of research activity are:

- Geology, Geophysics, and Earth Dynamics, including seismology and rock mechanics
- Geochemistry, including geochemical migration, brine and magma properties, and organic geochemistry
- Energy Resource Recognition, Evaluation, and Utilization, including underground imaging and the Continental Scientific Drilling Program
Solar-Terrestrial/Atmospheric Interactions

Emphasis is given to those aspects of the above activities of highest scientific priority and agency mission relevance. For example, several of the Geosciences Research projects involve advanced methods for remote sensing and measurement of the properties of earth materials. As an illustration, an ambitious project is now underway involving DOE's Sandia Laboratories and industrial support from oil companies. This work features the use of a DOE invention that measures stress in underground formations by exploiting an elastic strain recovery. Measurements are being made on cores obtained by drilling from platforms in the North Sea. Stress measurements will be applied to the problem of subsidence due to the extraction of petroleum. Platforms in one oil field have subsided more than 3 meters, and if this continues the platforms will have to be raised at a cost of hundreds of millions of dollars. The initial results from these measurements are leading both to practical results and to an improved understanding of the variations in the directions and magnitude of stress in a variety of rock types.

In addition to support of individual research projects, Geosciences Research emphasizes major integrated efforts with about one-third of its budget currently focused on the DOE portion of the national Continental Scientific Drilling Program. This national program is closely coordinated among the involved agencies under the terms of the Interagency Accord on Continental Scientific Drilling signed by DOE, the National Science Foundation, and the U. S. Geological Survey. Under the terms of the Accord, DOE is responsible for the drilling and logistic activities associated with thermal regimes (i.e., regions of abnormally high heat flow), although each agency supports research on such projects as may be consistent with its range of interests and capabilities. Since 1983, DOE has been leading the way in continental drilling with projects for obtaining core samples at the Salton Sea and
Long Valley in California and at the Valles Caldera in New Mexico. The organic geochemical processes—migration in the earth's crust; origin; maturation, migration, and entrapment of fossil energy resources—also are being studied and given increased emphasis, with special attention to research relating to domestic oil and gas resources. Such knowledge is essential if fossil fuels are to continue to be effectively exploited in the U.S.; it is also needed in dealing with the problems associated with toxic organic wastes.

More information on this subprogram can be obtained from James S. Coleman, Director, Division of Engineering and Geosciences, Office of Basic Energy Sciences, Department of Energy, Washington DC 20545, (301)353-5822. There are two reports available which supply more detailed information:


Advanced Energy Projects

The Advanced Energy Projects Division administers both the Advanced Energy Projects subprogram and Heavy Ion Fusion Accelerator Research (HIFAR).

The objective of the Advanced Energy Projects (AEP) subprogram is to explore the feasibility of novel energy-related concepts evolving from basic research which are at an early stage of scientific definition and, therefore, would not be of interest to technology programs. To qualify for AEP support, such concepts, even though they involve a high degree of risk, must have the potential for an eventual high payoff.

Advanced Energy Projects also sponsors exploratory research on concepts that do not readily fit into the existing DOE program structure. An area of major attention is the transfer of successful projects to technology programs; a number of such transfers have already been made. One, relatively recent, involved a new approach to "cryocooling," i.e., cooling matter to very low temperatures, close to absolute zero. Refrigeration to such temperatures is a highly energy-intensive process, widely used in the production of liquified gases such as helium, hydrogen, oxygen, nitrogen, etc. A technique known as "magnetic refrigeration" has been identified as having the potential for reducing energy consumption in the refrigeration process. A particularly clever embodiment of that technique was explored over the past few years by a group of researchers from Los Alamos National Laboratory (LANL).

With AEP funding, they constructed a laboratory-scale device which performed so well that the group, three people, was hired by a major manufacturing company (Astronautics Corporation of America) to develop a commercial model of the cryocooler. By September 1986, 15 scientists, engineers, and technicians at Astronautics were working toward the development of an engineering prototype.

Except under very unusual circumstances, Advanced Energy Projects supports individual projects for a limited time only. It differs from other subprograms in that it does not fund ongoing, evolutionary research. After a period of concentrated effort, typically about 3 years, the concept is expected to have proved itself, in which case the basic research phase is completed and the project can be transferred to a technology program. If a successful conclusion to the research is not foreseeable, the project is closed out.

Projects are selected from applications received from researchers at universities, industrial laboratories (including small R&D companies), and national laboratories.

Advanced Energy Projects is an interdisciplinary program whose projects cover a broad technological spectrum, e.g., new approaches to controlled fusion, new heat engines, novel methods for materials separations, new approaches to X-ray generation, including free electron and X-ray lasers, and new methods of accelerating particles.

A recent accomplishment of this subprogram was the first demonstration, in 1984, of a laboratory-size X-ray laser. More recently, in 1985, a successful use of mirrors to enhance the X-ray radiation, was achieved. There are many uses envisioned for the high-intensity, laser produced X rays in
medicine, physics, biology, and technology. In medicine, for example, the finely focused X-ray laser would allow better pinpointing in the use of CAT scanners and other devices aimed at specific body organs, cancerous tissues, or tumors.

Two activities, which involve promising approaches not supported elsewhere, are being pursued in the area of controlled fusion. One is called “muon-catalyzed fusion,” an intriguing option making use of the muon, a particle with the same electrical charge as an electron but 200 times heavier, to substantially increase the probability of a sustained fusion reaction at close to room temperature. This work is at a stage of early exploration. The other, mentioned earlier, is heavy ion fusion.

**Heavy Ion Fusion**

The Heavy Ion Fusion Accelerator Research (HIFAR) program is a spinoff from high-energy accelerator physics. The heavy ion fusion concept has grown out of inertial fusion research, which has been looking at different types of laser and particle beams, or “drivers,” that could be directed at targets—tiny pellets of deuterium and tritium—to achieve a fusion reaction.

Heavy ion beams would be attractive as an inertial fusion driver for generating energy if the uncertainties associated with accelerating heavy ions to the beam intensity required to drive a fusion reaction in the pellet could be successfully resolved. The HIFAR program goal over the next several years is to establish a data base in accelerator physics and technology that can allow the promise of the accelerator approach to be assessed accurately. Most of the current research activities in the HIFAR program are conducted at the Lawrence Berkeley Laboratory and the Los Alamos National Laboratory.

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 important to DOE's efforts in renewable resource production of fuels and chemicals, microbiological transformation of organic materials for conservation, and biological systems for resource recovery. The research is aimed at gaining an understanding of the underlying mechanisms of green plant productivity, converting biomass and other organic materials into fuel and chemicals by novel and improved methods of fermentation, and developing biosystems capable of saving energy.

Energy Biosciences research is focused on understanding 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 biochemical pathways and their genetic and biochemical regulation relating to degradation of abundant materials such as cellulose, hemicelluloses, and lignins and the conversion of these materials to fuels or chemicals are studied.

Microorganisms that grow in the absence of oxygen and are able to carry out fermentation with high efficiency are of special interest, as are thermophilic microorganisms, which have 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 to facilitate the production of fuels or petroleum-conserving chemicals or to yield biotechnologies capable of conserving energy.

A recent accomplishment under this subprogram involved the metabolic pathway leading to methane production from carbon dioxide. This pathway, including the major intermediates, enzymes and cofactors, has now been elucidated. During the biochemical reduction of carbon dioxide to methane, the carbon remains bound to carrier molecules called cofactors. The cofactors have only been found in bacteria which produce methane. (The cofactors are methanofuran, tetrahydromethanopterin, and thioethane sulfonic acid.) The presence of the enzymes responsible for these conversions has also been demonstrated. This work constitutes a major contribution to man's understanding of a major biological process of the carbon cycle in nature and one that has been harnessed to produce methane gas (a fuel).

This research into the physiology, biochemistry, and genetics of microorganisms and plants is carried out primarily at university laboratories.

Further information can be obtained from Robert Rabson, Director, Division of Energy Biosciences, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545, (301)353-2873. Also available is the Annual Report and Summaries of FY 1986 Activities (DOE/ER-0291), September 1986, which provides detailed descriptions of ongoing activities.

*The Energy Biosciences subprogram was formerly known as the Biological Energy Research subprogram.
Carbon Dioxide Research

Detailed worldwide measurements indicate that the amount of carbon dioxide (CO₂) in the earth's atmosphere is gradually increasing. Scientific analysis suggests that this increase could have substantial effects on climate, on agriculture, and on other human endeavors.

The goal of the Department of Energy's Carbon Dioxide Research Program is to improve the scientific knowledge base of the atmosphere, the biosphere, the oceans, and the cryosphere—their interactions and the effects that increasing atmospheric CO₂ and other trace gases will have on them. Accurate scientific data enable researchers to:

- Project future atmospheric CO₂ concentrations
- Estimate CO₂-induced global and regional climate changes
- Estimate crop and ecosystem response to higher CO₂ concentrations
- Evaluate human health and welfare effects attributable to CO₂-induced climate and vegetation changes

With a sound scientific knowledge base, it should be possible to conduct analyses of risk and cost/benefit so that potential options to aid decision making can be based upon a comprehensive understanding of CO₂-induced changes, and strategies by which we can modify and/or adapt to these potential changes.

Since 1977, significant research has been carried out by the United States and the international scientific community. The Department of Energy (DOE), the lead United

---

Fig. 2 Schematic diagram of the global carbon cycle.
States agency in the study of CO₂, and other agencies, including the National Science Foundation, National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, United States Geological Survey, United States Department of Agriculture, and Environmental Protection Agency, have conducted and supported research activities in universities, national laboratories, industry, and other institutions.

Looking forward to the 21st century, the DOE felt it was important to "take an accounting" to see how far this considerable effort had progressed toward answering the questions that had been posed in 1977 and in determining future research directions. Accordingly, the Carbon Dioxide Research Division published the following four state-of-the-art reports in 1985:

- *Atmospheric Carbon Dioxide and the Global Carbon Cycle*—the sources, reservoirs, and exchanges of carbon between all components of the global carbon system—the atmosphere, the biosphere, and the oceans (DOE/ER-0238).
- *Projecting the Climatic Effects of Increasing Carbon Dioxide*—the magnitude and rate of potential climate changes from increasing atmospheric CO₂ (DOE/ER-0239).
- *Detecting the Climatic Effects of Increasing Carbon Dioxide*—changes in climate resulting from increased atmospheric CO₂ distinguished from those caused by other factors (DOE/ER-0235).
- *Direct Effects of Increasing Carbon Dioxide on Vegetation*—plant response to increased atmospheric CO₂ and predicting crop and ecosystem response to CO₂ enrichment (DOE/ER-0238).

A focused research program continues to develop the scientific knowledge base to aid in analyzing possible energy policy options related to potential CO₂ effects.

Additional information about this subprogram is available from Frederick A. Koomanoff, Director, Carbon Dioxide Research Division, ER-12, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545, (301)353-3281. An annual report, *Carbon Dioxide and Climate: Summary of Research in FY 1986* (DOE/ER-0299), October 1986, also is available for more detailed information on this subprogram.

*These reports all can be obtained from the National Technical Information Service (NTIS), Springfield, VA 22161.
Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program, which is mandated by the Small Business Innovation Development Act of 1982 (P.L. 97-219), supports research and R&D activities at small business enterprises. DOE’s 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 the following: to stimulate technological innovation; to use small businesses 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 proposals 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 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 II 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, which specifies that agencies subject to this law, of which there are a dozen at present, including DOE, spend certain percentages of their extramural research or R&D funds on SBIR projects. The law specifies 1.25 percent for each fiscal year from 1986 through 1988. On this basis, the DOE budget for SBIR is approximately $29 million in FY 1986. 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 over two dozen topical areas. The slate of topics is changed somewhat from year to year, so as to offer, in time, a more complete representation of DOE’s wide range of interests in non-defense research related to its mission. The topics cover 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 4 years of the program, 1983-1986, 4138 Phase I proposals were received and 418 Phase I awards were made; 142 Phase II awards were made through FY 1986. The award selections have been made on the basis of scientific and technical excellence of the proposals.

Additional information about this program is available from Ryszard Gajewski, SBIR Program Manager, Department of Energy, Washington, DC 20545, (301)353-5995. Reports containing abstracts of the projects receiving support are available. The current reports are Abstracts of Phase I Awards, 1986 (DOE/ER-0285), and Abstracts of Phase II Awards, 1985 (DOE/ER-0209/1). The most recent program solicitation can be obtained by contacting the SBIR Program Manager.
Basic research in most areas pertinent to the DOE mission requires highly complex equipment and facilities. As mentioned earlier, the construction and operation of such facilities is costly, but many research projects depend on their availability. Basic Energy Sciences currently operates a number of facilities that are unique in the United States and, in some cases, in the world. The major BES facilities are described and discussed in the following subsections.

**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. The manner in which 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 that 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:

- Structure and dynamics of magnetic materials
- Dynamics of materials as they change phase
Neutron irradiation effects on the physical properties of materials
- Molecular structure and dynamics of organometallics
- 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
- 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 $1.1 \times 10^{15}$ neutrons/cm$^2$-sec available for research. Use of the HFBR facilities is divided between Participating Research Teams (PRTs) and general users. PRTs consist of scientists from BNL or other government laboratories, universities, and industrial labs 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 PRTs 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 remainder 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 $2.4 \times 10^{15}$ 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.

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

**High Flux Isotope Reactor**

**Oak Ridge National Laboratory**

**Oak Ridge, Tennessee**

The High Flux Isotope Reactor (HFIR) has a 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 $5 \times 10^{15}$ 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-gal drum and is replaced after about 3 weeks of operation. In addition to isotope production activities and in-core irradiations, there are 12 research stations at the 4 experimental ports. The National Center for Small Angle Scattering Research associated with the HFIR is sponsored as a joint project of DOE and the National Science Foundation.

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

- Magnetic properties of matter
- Lattice dynamics
- Defect-phonon interactions
- Lattices in superconductors
- Liquid structures
- Crystal structures

A wide variety of neutron scattering instruments have been constructed at the 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 on the basis of full cost recovery, including a charge for beam time.

An example of the broad capabilities made possible by the HFIR is recent research using neutron scattering to study the collagen spacing in mineralized bone. Collagen is a long chain-like molecule and is the principal organic component of bone, constituting about 30% of its weight. The collagen forms a regular array whose spacing can be measured by X-ray diffraction in demineralized bone.
The strength of the bone is provided by minerals which cross-link the collagen molecules preventing them from sliding by each other and thus hold the bone rigid. The collagen spacing, however, cannot be studied by X rays in mineralized bone because X rays are strongly absorbed and scattered by the much heavier mineral component. But the collagen spacing is easily observed in mineralized bone by neutron diffraction because neutrons are not strongly affected by the mineral. Study of the collagen in bone is essential to understanding mineral deposition in bone formation and mechanisms that cause mineral loss or osteoporosis. Results obtained so far demonstrate how mineral cross-linking takes place in bone formation and how it can be inhibited. Studies of the effect of vitamin C on bone formation and studies on the mechanism of osteoporosis are also under way. This research has involved several visiting as well as Oak Ridge scientists.

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, transplutonium 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. These sales, at full cost recovery, have resulted in revenues to HFIR of about $600,000 to $800,000 annually.

In FY 1985 total HFIR operating costs were about $8.5 million, of which about $1.4 million was defrayed by non-BES user research programs and radioisotope sales. BES-supported research activities at HFIR in FY 1985 were approximately $2 million. Other research at HFIR is supported by the Fusion Energy and Nuclear Energy Programs, the Nuclear Regulatory Commission, and the National Science Foundation.

Additional information about HFIR can be obtained from R. McCord, Operations Division, ORNL, Oak Ridge, TN 37831, (615)576-4991.

---

**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 electrons traveling in circular paths at very high energies). Synchrotron light radiation from the NSLS is continuous in spectrum, stable, 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 or 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 the use of synchrotron radiation to probe structure of matter but with capabilities well beyond those of X-ray and light sources previously available. Among the techniques used are many previously available but refined and extended to meet the opportunities provided by synchrotron radiation to study the structure and dynamics of matter. Techniques used 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 and has 28 photon ports, each able to handle one or more experiments. The vacuum ultraviolet (VUV) ring is 44 meters in circumference, with 16 photon ports. 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 and has achieved peak currents over 400 mA with average 100 mA lifetimes of more than 2 hours. The X-ray ring operates at 2.5 GeV.

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 (PRTs). The PRTs 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 (IDTs) to design and instrument beam lines and insertion devices. After an initial "commissioning period" to assure safety and reliability, NSLS and PRT beam lines become available for use by General Users. In the latter case, PRTs 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 surface 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
- Magnetic structure of surface and near surface layers in materials

In March 1986, a workshop was held at the NSLS site to explore a near-term practical application of synchrotron radiation. The Compact Synchrotron Technology Workshop attracted U. S. computer and semiconductor manufacturers interested in whether or not the use of small storage rings to manufacture integrated circuits would make them more competitive in the world market.

Representatives from firms such as AT&T, Texas Instruments, Hewlett-Packard, and IBM discussed the needs and specifications for a yet-to-be-built compact synchrotron to be used exclusively for X-ray lithography.

Semiconductor manufacturers are decreasing the size of the components of integrated circuits used in computers to increase their speed and capability. As the dimensions of capacitors, resistors, diodes, and transistors shrink below 0.5 micron, the use of ultraviolet light in a process called optical lithography to mass produce chips becomes more difficult. To make chips with more than 64 megabits of memory, shorter wavelength light, such as soft X rays, must be used in the lithography process.

In the process of lithography, radiation passes through openings in an opaque mask covering a transparent substrate. It "exposes" a polymer material called a resist that coats a semiconductor surface. When the resist is developed, it contains the pattern of the mask. Subsequent processing steps transfer the pattern to the semiconductor. The principal benefit of X rays, resolution, stems from the shorter wavelength of X rays as compared to the near ultraviolet radiation now used in optical lithography. For X-ray lithography, the mask is positioned about 40 micrometers above the semiconductor. Diffraction of the X rays and scattering of photoelectrons generated by X rays in the resist combine to give an optimum resolution in the neighborhood of 1000 angstroms.

The main advantage of synchrotron X-ray sources over conventional ones is the dramatically higher intensity. An exposure time of 1 sec, which is considered the maximum allowable for a manufacturing process to be economically competitive with the existing optical technology, demands much higher intensities. Also important, the small source size (0.1 millimeter at the NSLS), highly collimated radiation, and source-to-mask distance of several meters mean that for practical purposes the radiation from a synchrotron source is perfectly parallel and that the blurring effects due to a large source that radiates in all directions, which plague X-ray tubes, are much reduced.

The March 1986 workshop, the first of its kind in the United States, was BNL's response to the concern that individual U. S. semiconductor manufacturers would not be able to develop the compact synchrotron technology necessary to remain competitive in the world
computer chip market without the help of the storage-ring design experts at the national laboratories. Cooperation is necessary, however, if the U.S. semiconductor makers are to meet the challenge presented by the Japanese and West Germans, who are developing their own compact rings for X-ray lithography through government–industry partnerships.

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 authorized construction cost for NSLS ($24 million) provided for the building, storage rings, and a limited amount of experimental equipment for four of the beam ports.

A substantial amount of additional instrumentation and equipment has been installed, with private industry providing more than $10 million to date.

Additional information about NSLS can be obtained from Susan White-DePace, NSLS Department, Building 725B, Brookhaven National Laboratory, Upton, NY 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 SSRL, which shares the Stanford Positron Electron Electron Asymmetric Ring (SPEAR) with the High Energy Physics program, is an important research facility; at present it 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 available synchrotron radiation is provided 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.

Synchrotron radiation, the electromagnetic energy produced by relativistic electrons in magnetic fields, has many unusual properties that make it a most effective experimental tool. The SPEAR spectrum extends from the infrared through the visible, ultraviolet (UV), vacuum ultraviolet (VUV), and deep into the X-ray region. As a continuum source, synchrotron radiation is unrivaled. 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), and one 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 1000 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
- Development of a method of noninvasive angiography for heart disease patients

Most recently at SSRL a new X-ray beam line was started up that is an order of magnitude brighter than any other X-ray beam line in
the world. Initial experiments immediately demonstrated the unparalleled experimental capabilities of such high brightness beams. The structures of amorphous films as thin as 100 angstroms were studied using grazing incidence scattering.

The high brightness attained allows important new classes of experiments which have heretofore been impossible. The grazing incidence scattering experiments, for example, showed that it is possible to study thin poorly crystallized surface layers leading to the better understanding of such scientific and technologically important phenomena as oxidation, corrosion, and wear. Extreme brightness is required for several reasons: the samples’s cross section in grazing incidence is very small, the beam must be highly parallel to optimize surface sensitivity, and the amorphous materials are very weak scatterers. A number of non-SSRL “users”—AT&T Bell Labs, Exxon, BNL, Hewlett-Packard, and Stanford University—as well as SSRL staff have been involved in this work.

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
- Noninvasive angiography
- X-ray lithography and microscopy

SSRL serves approximately 500 scientists from 124 institutions working on more than 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 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.

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

Intense Pulsed Neutron Source

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 high fluxes of neutrons in bursts that are precisely in step with the 30-Hz frequency (a 30-Hz frequency means there are 30 bursts per sec) 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
- 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
- Radiation damage at cryogenic temperatures

Two principal types of scientific activity are underway at IPNS:
(1) 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 (2) 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 measurement as well as for technological applications, such as to measure stress distribution in materials and characterization of zeolites, ceramics, and hydrocarbons.

Recently, through use of the IPNS, a new technique for study of surface magnetization, Polarized Neutron Reflection, was developed. It is a nondestructive method for direct microscopic probing of the magnetism in surface layers and has been successfully used to map field penetration in superconductors and magnetic depth profiles in prototype recording devices utilizing layered magnetic materials.

This is the first nondestructive technique that can provide microscopic magnetization information over the range 20Å-500Å from a surface. In basic research it is the only method to directly test theories of surface phenomena in superconductivity, and, despite 50 years of effort in this area, unexpected behavior was seen in lead-bismuth alloys. This work is having a major impact on the theory of superconductivity. In applied research it is likely to prove revolutionary in characterizing magnetic multilayers.

The IPNS, which began operation in FY 1981, has a peak thermal flux of $3 \times 10^{14}$ 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 $2 \times 10^{12}$ neutrons/cm$^2$-sec. The proton current is 8 microamps providing 500 meV protons in 30 bursts per second of $2 \times 10^{12}$ 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 ultracold 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.
Los Alamos Neutron Scattering Center

Los Alamos National Laboratory
Los Alamos, New Mexico

The Los Alamos Neutron Scattering Center (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, $1.7 \times 10^{16}$ 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.

When the LANSCE facility is completed, it 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 nonsensitive countries. DOE approval is required for any other foreign national visits.

Available instruments are: (a) 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) 667-6669.

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

Scientists at the CRF have recently developed a process,
called RAPRENOx, for the removal of nitrogen oxides from automotive exhaust gases. The process was discovered while carrying out fundamental studies of the combustion chemistry of nitrogen. The feasibility of the process was demonstrated by using it to effect the removal of nitrogen oxides from the exhaust of an experimental diesel engine. This process is one in which an inexpensive substance is added to the exhaust stream from a combustor. The starting material is cyanuric acid, commonly used for water treatment in swimming pools. The RAPRENOx process has been studied in laboratory kinetics experiments and has been successfully demonstrated using a diesel engine. It is believed that RAPRENOx will be broadly applicable to combustion exhausts. A patent application was filed for the process, and a waiver of patent rights was granted to the inventor in the interest of fostering rapid commercialization in the private sector.

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 scientists 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 14 individual research laboratories, 4 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, CA 94550, (415) 422-2520.
High-Voltage and Atomic Resolution Microscope Facilities

High-Voltage Electron Microscopes (HVEMs) are invaluable for energy-related research important to, e.g., fission and fusion (radiation damage), conservation and fossil (high-strength steel and high-temperature ceramics for automotive turbines), fossil (corrosion), and solar (photovoltaics) technologies. The microscopes are also important for general research, and each institution having one has developed or is developing a sizeable outside user group of academic and industrial scientists.

The HVEM is useful for transmission electron microscopy of heavy metals, studies that must use "thick" samples to avoid surface effects, and studies of brittle materials, such as ceramics, which are difficult to prepare in thin form. Also, high-voltage machines are necessary for materials studies incorporating special environments and for in-situ radiation damage studies. It is possible to "see" damage as it is being produced.

Basic Energy Sciences supports three facilities with HVEMs and the atomic resolution microscope (ARM), which came on-line in 1983.

National Center for Electron Microscopy

Lawrence Berkeley Laboratory
Berkeley, California

The National Center for Electron Microscopy (NCEM), which cost $8.0 million dollars, was dedicated on September 30, 1983. The Center contains the most advanced electron microscopes in the world and has as its centerpiece the only atomic resolution electron microscope (ARM) in the United States. Besides the ARM, other available microscopes are a Hitachi HU-650, a Kratos EM-1500, and JEOL 200 CX.

The Atomic Resolution Electron Microscope (ARM) was specifically designed for optimum performance in the high-resolution imaging mode. Attention has been given to the potential problem of specimen sensitivity to the electron beam at high accelerating voltages, and instrumentation was incorporated so that the microscope could operate with minimum aberration over its entire voltage range (400 to 1000 KeV). At its maximum voltage (1 MeV), the ARM has a point-to-point resolution of 1.7Å (although 1.5Å has been achieved). The microscope also can be run in a mode that enables convergent beam electron diffraction (CBED) patterns to be taken from the same specimen areas imaged in high resolution. An example of the capabilities of this machine is shown in the photograph on page 39 of a germanium precipitate needle, viewed end-on in an aluminum matrix, resolving the atomic positions for both elements.

The Kratos EM-1500 HVEM is designed primarily for dynamic in-situ studies, but it can also resolve structures at the 3Å level. It provides accelerating voltages of 1200 to 1500 KeV, which are not available elsewhere in the United States.

A support instrument to the ARM, the JEM 200-CX is a high-resolution machine with a maximum operating voltage of 200 KeV and a point-to-point resolution of about 2.4Å. Specimens for this microscope are restricted to 2.3 mm in diameter to fit into the ultrahigh resolution pole piece.

The fourth microscope at LBL is the Hitachi HU-650. It has an accelerating voltage that is continuously variable between 200 and 650 KeV but most conveniently used at three fixed voltages: 300, 500, or 650 KeV. The resolution limit of this instrument is not high (about 20Å) but it is adequate for some studies, exploratory experiments, and many hot stage or environmental cell experiments.
High Voltage Electron Microscopy-Tandem Facility

Argonne National Laboratory
Argonne, Illinois

The High Voltage Electron Microscope (HVEM)-Tandem Facility provides unique combinations of the techniques of a high-voltage electron microscope, ion implantation/bombardment, and ion-beam analysis. In addition, the HVEM/ion-beam interface permits direct observation of the effects of electron and ion bombardment on materials in the microscope. Current experimental studies using the HVEM represent a wide range of materials research from universities, national laboratories, and industry. Work includes programs in mechanical properties, corrosion and oxidation, radiation damage, and general defect analysis.

The principal components of the HVEM-Tandem Facility are a Kratos 1.2-MeV high-voltage-transmission electron microscope with ion-beam interface, a National Electrostatics 2-MeV tandem-type universal ion accelerator, and a Texas Nuclear 300-KeV ion accelerator. These two accelerators together provide ion beams of essentially all elements from ~10 KeV to 8 MeV.

The high-voltage electron microscope has a maximum voltage of 1.2 MeV and a demonstrated lattice resolution of 3.5Å. The microscope contains a number of unique features including 100- to 1200-KeV continuous-mode voltage selection. Special specimen rods for viewing and for measuring the intensity of the ion beam within the microscope are available, and observations can be made at temperatures between 10 and 130°K in high-vacuum conditions.
Observations in gaseous atmospheres at pressures of up to $2.5 \times 10^4$ Pa can be carried out between ambient temperature and 1300°K using a gas reaction cell inserted into the specimen chamber. The 2.0-MeV Tandem Accelerator has an internal and two external negative sources for helium and metal ions; it can generate ions of all stable isotopes in the periodic table. The accelerator can be operated in conjunction with the HVEM or separately for ion implantation/bombardment and ion-beam-analysis studies. Typical ion-beam currents will range from $\sim$10 amperes for protons to 0.1 µA for $^{204}$Pb$^+$. The 300-KeV ion accelerator has been equipped with sources for metal and gaseous positive ions. It can be used in conjunction with the ion-beam interface when lower-energy ions are required or to deliver ions into two of the target chambers of the Tandem system for ion implantation studies.

### Shared Research Equipment Program

**Oak Ridge National Laboratory**
**Oak Ridge, Tennessee**

The Shared Research Equipment program (SHaRE) is a collaborative program in which personnel at Oak Ridge National Laboratory work with scientists from other institutions. The purposes of the program are to provide university and industrial researchers with access to equipment for microstructural analysis that is not available at their home institutions and, in so doing, to facilitate additional laboratory research that would not otherwise be accomplished. The laboratory staff shares with visitors responsibility for both completing the project and ensuring publication of the results.

A number of major instruments are available to collaborators. Nuclear microanalysis and Rutherford back-scattering analysis are performed in two separate systems, and four variously equipped 120-KeV transmission electron microscopes are in service. A Hitachi 1-MeV HVEM is equipped for environmental and mechanical deformation investigations. Two Auger analysis systems, one with scanning capability, also belong to the equipment pool in the SHaRE program.

### Calutrons-Electromagnetic Isotope Separations Facility

**Oak Ridge National Laboratory**
**Oak Ridge, Tennessee**

The electromagnetic isotope separations facility at Oak Ridge National Laboratory (ORNL) is not a user facility in the normal sense. It is used to enrich stable isotopes, selected radioactive isotopes, and heavy-element isotopes for use in research and development and in commercial activities. It consists of very high current mass separators, known as Calutrons, which were originally designed and built under the Manhattan Project during World War II. The Calutron facility is a unique national asset; the USSR is the only other nation possessing such a facility. Many other countries have laboratories in which isotopes are enriched, but these facilities are usually of limited size, and the isotopes are used for specific purposes. The ORNL Isotope Distribution Office makes isotopes available in two ways: Multigram quantities of enriched samples from the "Research Materials Collection" are "loaned" at a nominal fee to members of the DOE research community for nondestructive research, and enriched isotopes are sold to other research and commercial organizations on a cost-recovery basis.

The facility is illustrated in the photo on the opposite page. It consists of two "tracks" containing separator tanks. Eight tanks are reserved for chemically hazardous and radioactive elements and 44 for stable isotopes. Of these, 30 comprise the stable isotope track (the foreground). Ten remaining tanks can be used to separate either radioactive or stable isotopes. It is possible to enrich the isotopes of four elements simultaneously in the 30 Calutrons of the stable isotope track.

When feed material, in elemental or compound form, is introduced into a Calutron, it is either directly vaporized or heated with chemical treatment to form a volatile species. This vapor is then
ionized. The ionized particle of the element being separated is extracted from the ion source, accelerated, and magnetically focused. The focused individual isotopic beams are intercepted by collectors constructed of carbon, copper, or aluminum. After a run, which may be fifty to several hundred hours depending on the element, the collectors are removed from the separator, and the material is extracted, chemically purified, assayed, and placed in the inventory.

Since each element or compound has unique operating characteristics, it is difficult to generalize about the throughput capability of the facility. As a rule of thumb, one separator can provide approximately 0.1 mole of an element per day of operation. This figure is multiplied by the natural isotopic abundance to determine the yield for a particular isotope. Isotopic purity depends on the natural isotopic abundance of the isotope required and the abundance of its nearest neighbors. The products of one separation can be recycled to obtain a significantly higher isotopic assay in a two-pass process.

Materials are available from the Research Materials Collection (RMC) for loan to U. S. scientists for use in nondestructive experiments and to non-U. S. scientists under restrictive conditions (e.g., the experiment must be of direct relevance to the DOE technology programs, such as the use of RMC samples within the European community for the study of neutron cross sections). Such loans are usually made only on the strong recommendation of the U. S. Nuclear Data Committee.

Materials are sold from the sales inventory to anyone on a first-come, first-served basis. Up-to-date information on the electromagnetically enriched isotopes, their chemical form, percent enrichment, price per milligram, and availability can be obtained from J. Setaro, Operations Division, ORNL, P. O. Box X, Oak Ridge, TN 37831, (615) 574-5903.
Transuranium Processing Plant

**Oak Ridge National Laboratory**  
**Oak Ridge, Tennessee**

The Transuranium Processing Plant (TPP) was built to recover radioactive transuranium elements from irradiated targets and to serve other chemical processing and fabrication needs of the Transplutonium Production Program of the Atomic Energy Commission. It is not a research facility for BES, but it provides unique chemical processing capabilities for highly radioactive actinide materials. It is integrally tied to the HFIR heavy element production activities and contributes to DOE's isotope production and sales activities. Research in nuclear chemistry and physics and nuclear technology is supported by TPP activities. A nuclear energy program "user" group was in residence at TPP operating the Solvent Extraction Test Facility, which is part of the ORNL Consolidated Fuel Reprocessing Program, through the end of FY 1986.

Samples ranging from hundreds of grams of curium-244 to picograms \(10^{-12}\) of fermium-257 have been provided by TPP, and research quantities of a variety of transuranium isotopes prepared at TPP have contributed to our understanding of the chemical, physical, and nuclear properties of the actinide and higher elements.

The TPP, built at a cost of $8.8 million, began "hot" operation in 1966. It contains seven hot cells, each equipped to carry out remotely one or more separate procedures for chemical separation, purification, fabrication, or analysis of highly radioactive materials. Additional information can be obtained from L. King, Chemical Technology Division, ORNL, Oak Ridge, TN 37831, (615) 574-7071.
Basic Energy Sciences (BES) and its predecessors have funded and conducted basic research programs in the physical and related sciences and managed complex national facilities since the 1940s, 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, thereby providing the nation a knowledge base and source of new technology to maintain a healthy economy. Basic Energy Science's 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 for specific individual energy technology options is extremely important, so also is our need for basic research to build the science base independent of those technologies we currently perceive will be important several decades from now. It is from such basic research and its generation of new ideas and concepts that radical improvements in currently identified options or entirely new options may emerge.

Since 1984, the following Basic Energy Sciences Program and Budget Trends have emerged:

- 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.
- Initiation of a program to develop advanced scientific facilities for research of importance to the nation where the expertise lies primarily at DOE national laboratories.

The budget for FY 1986 is approximately $432 million (Table I) of which $25.7 million, ~6%, is for capital equipment. The fraction of the FY 1986 budget appropriation designated for construction is 16%.

Some changes in responsibility occurred during FY 1986. Support for Heavy Ion Fusion Research, which has been managed under the Nuclear Physics activity and budgeted in the Nuclear Sciences subprogram at a level of $5 million, is now included within the Advanced Energy Projects subprogram. Also in FY 1986, several new construction projects were undertaken at the initiative of the Congress to provide updated, modern buildings for research on university campuses. They are at the University of Alabama, Tulane University, Atlanta University, and Brown University. Several other university construction projects undertaken previously and continuing in 1986 are at

### TABLE I
Office of Basic Energy Sciences Budget

<table>
<thead>
<tr>
<th>FY 1985 10^6 dollars</th>
<th>Estimated FY 1986 10^6 dollars</th>
<th>Congressional request FY 1987 10^6 dollars</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating Expenses (by subprogram)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Materials Sciences</td>
<td>132.2</td>
<td>132.6</td>
</tr>
<tr>
<td>Chemical Sciences</td>
<td>103.9</td>
<td>104.3</td>
</tr>
<tr>
<td>Applied Mathematical Sciences</td>
<td>34.5</td>
<td>37.4</td>
</tr>
<tr>
<td>Engineering and Geosciences</td>
<td>26.1</td>
<td>25.3</td>
</tr>
<tr>
<td>Advanced Energy Projects</td>
<td>14.8</td>
<td>11.8</td>
</tr>
<tr>
<td>Energy Biosciences</td>
<td>12.4</td>
<td>11.8</td>
</tr>
<tr>
<td>Carbon Dioxide Research</td>
<td>13.1</td>
<td>12.4</td>
</tr>
<tr>
<td>Program Direction</td>
<td>3.8</td>
<td>3.5</td>
</tr>
<tr>
<td>Subtotal</td>
<td>340.8</td>
<td>339.1</td>
</tr>
<tr>
<td>Capital Equipment</td>
<td>31.1</td>
<td>25.7</td>
</tr>
<tr>
<td>Construction</td>
<td>42.4</td>
<td>67.5</td>
</tr>
<tr>
<td>Total</td>
<td>414.3</td>
<td>432.3</td>
</tr>
</tbody>
</table>
Columbia University and the University of Oregon. In addition to these projects, work continued on an expansion of the National Synchrotron Light Source, the Stanford Synchrotron Radiation Laboratory, and the Center for Advanced Materials at the Lawrence Berkeley Laboratory.

Figure 3 presents a breakdown identifying the major performers who carry out the Basic Energy Sciences program. About 67% of the program is conducted at the national laboratories including Lawrence Berkeley Laboratory (LBL) and Ames Laboratory, 30% at universities throughout the country, and the remainder elsewhere, including nonprofit institutions and industry.

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 17% 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 post-doctoral students.

Of the funding going to national laboratories, about 90% is for activities uniquely dependent on the facilities and services specific to each laboratory. The operation of major scientific facilities continues to require a large commitment of BES funds. Operating costs for BES's major user facilities for FY 1986, exclusive of the costs of research at them, are projected at $54 million; they are expected to rise to $63 million in FY 1987.

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,

Fig. 3 Breakdown of research by (a) performers and (b) nature of activities at national laboratories.
and strengthening of research in the areas of science dealing with:

- Surfaces—modification, interfaces, reactions at surfaces
- Solids—properties and structure, including grain boundaries, condensed matter theory, atomic transport, amorphous materials, structural ceramics
- Plants—genetics, response to stress, photochemistry
- Geothermal energy resources—occurrence, characterization, chemical and thermal properties
- Multiphase systems—transport properties, chemical behavior, etc
- Chemical reactivity, photochemistry, photosynthesis, catalysis

Experiments with, for example, phenomena involving extremely short time periods, vanishingly small concentrations of reacting species, entities with only transient existence, and measurements under extreme conditions of temperature and pressure point out the necessity for constantly improving equipment. Examples of BES's efforts to meet these kinds of challenges include the new Atomic Resolution Microscope and the ever increasing efforts to exploit synchrotron radiation and advanced neutron sources to increase our understanding of the atomic structure of materials. Despite increasing costs and demands for constantly improved equipment and installations, the unique research programs and facilities supported by BES must be maintained, improved and expanded. The knowledge base they create is vital to improving or developing new energy technologies and maintaining U. S. competitiveness.