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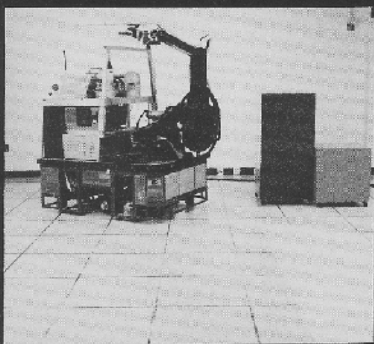
October 1990

U.S. Department of Energy
Office of Energy Research

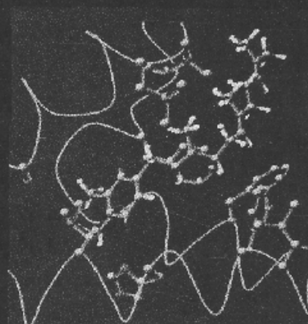
BES

Office of Basic Energy Sciences

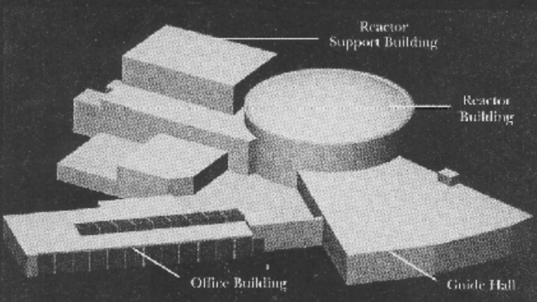
1990 Summary Report



Smart Robot



Photosynthesis Protein Model



Advanced Neutron Source

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1990 Summary Report

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

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

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Introduction

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

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

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

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

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

Overview

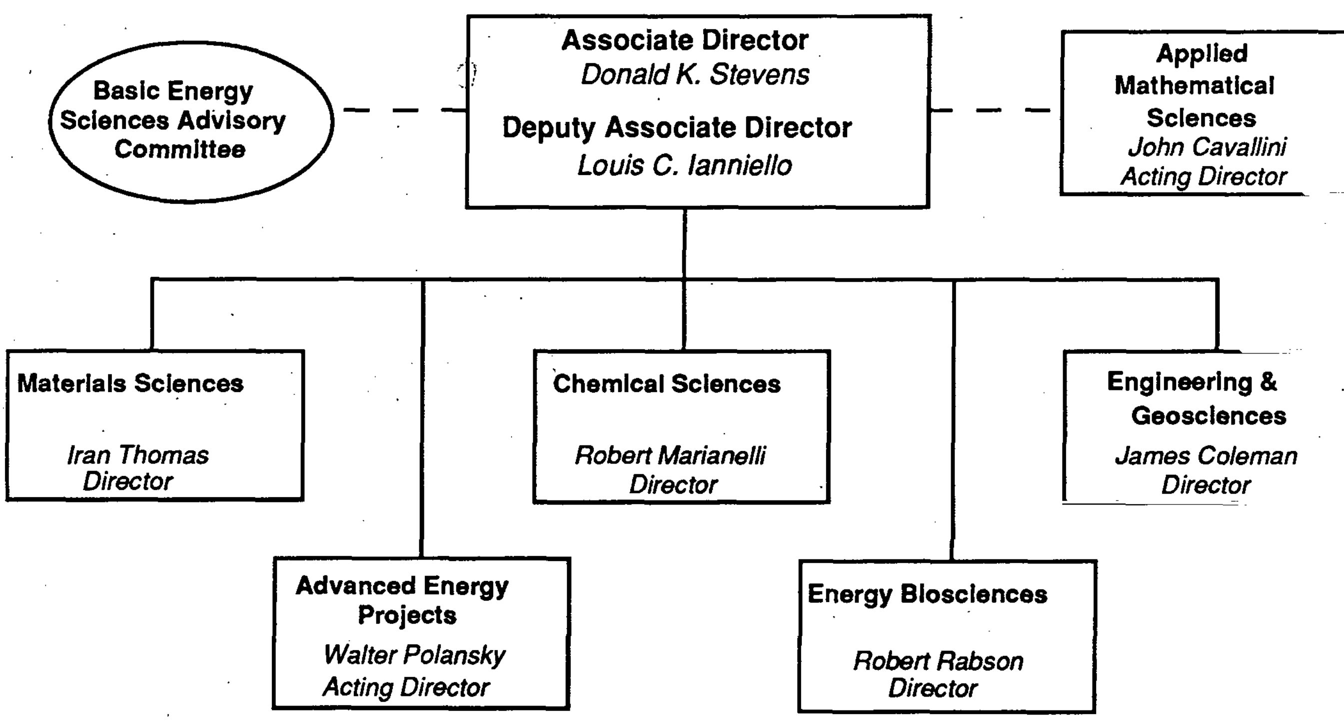
Basic research requires long-term commitments of resources and people with the promise only of long-term success and long-term return on investment. Thus, the private sector, dominated by concerns for high and rapid return on investment and other short-term considerations, is playing a lesser role in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

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

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

Figure 1.

Office of Basic Energy Sciences



mechanical fracture involving both Materials Sciences and Engineering and Geosciences subprograms.

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

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

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

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

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

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

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

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

- *Surfaces*: behavior and properties at the atomic and molecular level, chemical reactions at surfaces and modifications to them, and behavior and properties at interfaces.
- *Solids*: their properties and structures at the atomic and molecular level including grain boundary effects, electronic and magnetic properties, and atomic transport within solids. Of particular interest are condensed matter theory, structural ceramics and amorphous -- glassy or plastic -- materials.
- *Plants*: including genetics; response to stress, i.e., their ability to adapt to low moisture, high-temperature, high-salinity, etc., environments; and photochemistry -- the effect of sunlight on the internal chemistry of plants including photosynthesis and the complex reactions involved.
- *Rock/Fluid Systems*: geophysics and geochemistry of systems relevant to energy resource recovery and isolation of energy-related wastes, including topics such as underground imaging, flow in fractured reservoirs, and isotope geochemistry.

BES continues to emphasize interactions with U.S. industry. Recently this has included development of an activity that has come to be known as "Technology Transfer", operated through the national laboratories, to enhance the flow of research results to the private sector. Some examples of recent research results contributing towards early application are:

- ***Detection Devices for Trace Explosives and Pollutants*** -- A device to detect explosives was under development at the Oak Ridge National Laboratory during 1989; the concept for it grew out of an analytical research effort there under the BES program. This device is designed to detect trace gas components characteristic of explosive materials. Also based on this research, an exclusive license was granted to a private firm to develop a commercial device for detection of pollutants in the environment.
- ***Environmentally Safe Scavengers for Metal Contaminants*** -- Chemical compounds able to remove metal ions from acid streams have been developed which, once used, can then, without much difficulty, be turned into harmless substances: water, carbon dioxide, and phosphoric acid. These new compounds are efficient for removing metals and are expected to be quite useful for processing very acid nuclear wastes and for decontamination of ground water by removing metal ions from them. A patent application is being processed, and several firms have expressed interest in obtaining a license to produce these compounds on a commercial scale.
- ***Nobel Prize Work Leads To Commercial Products To Analyze Body Fluids***--In 1987, Professor Donald J. Cram, supported for many years by BES, shared in the Nobel Prize in Chemistry for "developing new chemical methods for recovering scarce metals and purifying

common metals using much less energy than in the past". Professor Cram's research provided new insight into the chemistry of selectively combining molecules which can "tie up" a valuable metal in the presence of other metals in solution. The novel complexing agents developed can bind molecules as well as metals and can be designed to mimic the highly specific activity of enzymes. In 1989, these complexing agents were adapted by a commercial firm for quantitative analysis of sodium and potassium, an important measurement for proper electrolyte balance in the human body. Such analyses are conducted routinely in the clinical laboratory.

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. To carry 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, and the establishment of electron microscopy centers.

As noted earlier (Figure 1), BES is organized along scientific discipline lines. Research is managed under six subprograms: Materials Sciences, Chemical Sciences, Engineering and Geosciences, Advanced Energy Projects, Energy Biosciences, and Applied Mathematical Sciences. The Applied Mathematical Sciences activities are managed by the Scientific Computing Staff, which reports directly to the Director, Office of Energy Research, but the activity is budgeted under BES. The "Subprogram" section describes the activities in each of the subprograms.

Special Topic

Basic Energy Sciences Support for Research Relevant To Environmental Concerns

Each year in the Basic Energy Sciences (BES) Summary Report, a special topic is selected and highlighted to give the reader an indepth look at how the BES program contributes to understanding in a particular field. The topic selected this year is research relevant to environmental concerns. Three stories are presented of research started decades ago which contributed to heightened environmental awareness and eventually to societal action to mitigate the concerns. They show the painstaking process involved in basic research and its unmistakable value to the issues of environmental quality. Additionally, this section includes four more recently initiated research projects in which areas of environmental interests are being actively pursued and which may, in the future, lead to equally important mitigation actions.

Since the end of World War II, the Office of Basic Energy Sciences and its predecessor organizations have been a principal source of support for basic research in areas leading to environmental awareness and providing the technical foundation for solutions to environmental concerns. For example, current sensitivity to environmental issues would not exist without our present capability to measure environmental pollutants and to identify those trace materials that pose major hazards to mankind. That capability would not exist if it were not for the painstaking research over the past four decades that constantly sought to make better, more precise measurements in smaller and smaller systems and to develop new techniques to understand the environment.

Originally responsible for basic research in the physical sciences, the early program was focused on radioactivity and radiation, understanding these phenomena and their origins, their effects, and potential applications to serve mankind. An important consequence of the concerns with radioactivity was learning to deal with trace quantities of materials, both handling them and measuring them, and using isotopes to tag certain chemicals. Thus, the analytical techniques had to be developed along with the research. The physical research program worked in close concert with its sister organization responsible for biological and medical research involving atomic energy. More recently, research has been initiated in engineering and geosciences with the expectation that discoveries here will have similarly significant impact.

Sensitivity to the undesirable impacts possible from trace amounts of radioactive materials, coupled with evolving analytical capabilities and continuing improvements in electronics and instrumentation, have had an important effect on science in general; on biology and medicine, particularly regarding trace materials in living systems; and on society. Society has become concerned with environmental issues to a degree unprecedented in man's history.

It is nearly impossible to trace the detailed evolution of environmental awareness, pinpointing the contributions made to it by this program. It is possible, however, to identify the generic aspects, and in several instances, the specifics, of BES-supported basic research contributions to societal awareness and actions to deal with environmental problems.

Generically, BES has supported the development of better and better analytical tools to identify minute quantities of trace materials; BES has supported research to elucidate chemical reactions and processes involving trace materials; and BES has supported theoretical research exploring possible reactions and behavior in systems of environmental concern.

Specifically, BES has contributed to the identification of leaded gasoline as a major environmental pollutant and, ultimately, to a national policy to reduce its use; BES has supported the research leading to the recognition of the long-term effect of chlorofluorocarbon release on the ozone layer which was then followed by international action to reduce that effect. Research BES has supported also has provided the information and capabilities needed to conduct analyses and assessments of potential hazards of proposed technologies. An example is the identification of the effect a fleet of supersonic transport (SST) aircraft might have on the ozone layer if pursued as a major transportation option for the United States. Professor Harold Johnston of the University of California, Berkeley, and Lawrence Berkeley Laboratory, raised the issue of the ozone layer in 1971 and Professor F. Sherwood Rowland, University of California, Irvine, shortly thereafter (1974) recognized and called attention to the chlorofluorocarbon-ozone chemistry that could affect the ozone layer. As more and more research is carried out and data obtained, the understanding of the ozone layer and the chemistry of the stratosphere improves; the concerns raised by Rowland have become widely accepted and led to international agreements and national policies aimed at reducing man's release of chlorofluorocarbons into the atmosphere*.

In addition to the above three stories which are focused on research begun many years ago and, hence, have developed complex interactions and results, included in this section are four items started more recently which may very well lead to equally complex, interesting stories some time in the future. They are: Global Geochemical Cycles and Climate Change; Use of Geophysical Methods for Environmental Studies; Use of Robots to Clean Nuclear and Chemical Wastes; and Underground Imaging and Borehole Technology.

The histories of the leaded gasoline, ozone layer, and SST-related research are important because each points out the value to society of the long-term basic research supported by BES. The environmental impact of the latter four more recent items and other research supported by BES is unknown, but judging from past experience, they will also contribute in a complex way to the solution of environmental concerns. The BES program, which is aimed at understanding phenomena of interest to DOE's energy technology and weapons programs, searches for added understanding of the fundamental behavior of matter and energy, including any effects on the environment in which we live. The ultimate achievement of these goals are tied to man's survival.

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* An article in American Scientist, January-February 1989, by Rowland, provides a fine review of the CFC-O_3 issue.

Leaded Gasoline

The identification of tetraethyl lead from automobile exhaust as the principal source of lead which has contaminated the earth's biosphere came about through basic geochemical research on lead in the earth's crust and its isotopic composition. That research, supported by the U.S. Atomic Energy Commission (AEC), pioneered the use of stable lead isotopes, which are the products of radioactive decay from uranium and thorium, as tracers to identify geologic processes and origins of crustal materials.

Different lead isotopes are produced at different rates depending on the abundances and radioactive half-lives of their uranium or thorium precursors. Over long times comparable to the earth's age, the relative abundances of different lead isotopes change. Such relative isotopic abundance changes, considered along with actual abundances of lead, uranium, and thorium in various kinds of rocks, provide a means for unraveling the ways in which the various parts of the earth's crust evolved during ancient times from the earth's mantle, as well as providing information about continental drift and paleotectonic evolution.

The rationale behind AEC's support of these pioneering basic scientific studies of the isotopic evolution of lead was that they helped establish fundamental knowledge of the origin, types, and magnitudes of reservoirs of uranium within the earth's crust. One of the initial findings from these studies was that enough uranium could be recovered from ordinary granite to produce nuclear fuel with an energy content well in excess of that needed to carry out the fuel recovery and production operations.

Of greater significance is the knowledge that people today contain 1,000 times more lead in their bodies than did their prehistoric ancestors, knowledge resulting from a discovery made while conducting basic research on the isotopic evolution of lead.

In 1962[1], T. J. Chow[2] and C. C. Patterson[3] reported on their research aimed at establishing the current mean isotopic composition of lead in the earth's crust. They approached the problem viewing ocean leads as suitable for their purpose, but this required that the answer be obtained indirectly from lead deposited at various geologic times in deep ocean sediments.

Experimental data presented was accompanied by interpretive arguments involving the nature and occurrence of lead in pelagic sediments*, the transport and origin of marine lead, its isotopic composition in relation to time of deposition, and the characteristics and meaning of the isotopic variations observed.

Using various data from the scientific literature and reasonable assumptions, quantitative estimates were made of the amounts of lead, uranium, and thorium transported to the seas either as particles or in solution in river waters, or by atmospheric transport. It was estimated that about two-thirds of the lead in sediments deposited in pelagic regions comes from soluble lead in ocean waters, not from particles. This chemical deposition of lead is a process that has operated for a long time. It results in the net removal of lead from uranium-lead-thorium systems in the continents and the storage of this lead in pelagic regions. The removal of continental lead tends to increase the relative proportion of young radiogenic lead in the continent above the ratio that would normally be found in a closed system.

Rates of accumulation of pelagic sediments had been previously identified by others. Chow and Patterson's work, obtaining lead concentration and isotopic data, coupled with rate of deposition data obtained by others, contributed to the clarification of the oceanic cycling of lead. As a result, transport mechanisms for lead from the continents to the marine environment were delineated and their magnitudes established. As a consequence of outlining the broader implications of oceanic leads as they apply to chemical oceanography and to the geochemistry of uranium, thorium, and lead in the earth's crust and mantle, Chow and Patterson determined the rate at which lead had entered the oceans, passed through them, and was deposited in sediments during ancient times.

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[1] T. J. Chow and C. C. Patterson, The Occurrence and Significance of Lead Isotopes in Pelagic Sediments, Geochimica et Cosmochimica Acta, 26, pp. 263 to 308, (1962). [AEC is credited as providing supplemental support for this work through a contract; most of the support was from the American Petroleum Institute (API) and there was a short term NSF grant.]

[2] At Scripps Institution of Oceanography when this paper was published.

[3] At California Institute of Technology when this paper was published.

* Pelagic sediments are those found in the open sea.

Most of the dissolved lead in the oceans originated from continental weathered rocks containing leads of various isotopic compositions, and about 10% of the amount that entered the oceans during the last million years may have originated from volcanic activity. The effect of industrial contamination, however, was thought to contribute dissolved lead to the oceans at a rate much greater than the average of the last million years, and much of the lead now in young ocean waters may be seriously contaminated by ore lead mined by man.

They pointed out from reported industrial production (mainly lead alkyls) that man is presently dispersing lead over the land surfaces at a rate of about 2.3 $x10^{12}$ grams per year. About one-third of this is exposed to the weathering cycle and is the source of lead entering the oceans from rivers. This is 80 times the rate of oceanic deposition of soluble lead from the oceans to sediments in the prehistoric past. Chow and Patterson concluded that effects of such industrial pollution totally obscured true magnitudes of cycles of lead in the oceans today.

The discovery of the gross discrepancy between large inputs of industrial lead to the oceans from air and rivers today compared to the much smaller outputs of natural lead from the oceans to the sediments in the ancient past was the key finding that triggered a series of subsequent investigations carried out during the next two decades which disclosed the serious problem of poisoning effects from industrial lead pollution which confronts most Americans today.

Concentrations of industrial lead in the earth's global atmosphere are 100 times greater than concentrations of atmospheric lead deduced from measurements of lead recorded in ancient polar snow layers.[4,5] More recent work by Patterson and others has further confirmed the effects of this increased introduction of atmospheric industrial lead in increasing amounts of lead on plant leaves and animal fur in remote ecosystems.

The basic scientific studies of biogeochemical cycles of lead in terrestrial and marine ecosystems, which were initiated and then supported in part by AEC funds, have provided a reliable foundation of knowledge upon which the economics of controlling industrial lead pollution can be based. These studies have also established new methods and concepts to allow a better understanding of how to monitor and control the escape of toxic substances from waste storage sites into ground water tables. For lead, for example, the isotopic compositions from industrial sources are generally different from the isotopic compositions of natural lead in soils, so they can be distinguished. This allows the flow of industrial pollutant lead, added to soils from air by lead-rich aerosols incorporated in rain and snow and by lead-rich aerosols deposited on plant leaves, to be followed as it percolates through soils into aquifers and streams.

In this way, lead was proven to be a unique, powerful tool for both tracing out the historical sequence of certain geological events and increasing our knowledge of the operation of the biosphere, the oceans and the circulation of ocean waters, but also for studying the perturbation by industrial pollution of the geochemistry of lead.

Later, using isotope dilution techniques, M. Tatsumoto and

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[4] M. Murozumi, T. J. Chow and C. Patterson, Chemical Concentrations of Pollutant Lead Aerosols, Terrestrial Dusts and Sea Salts in Greenland and Antarctic Snow Strata, Geochimica et Cosmochimica Acta, 33, 1247-1294 (1969) (AEC support).

[5] A. Ng and C. C. Patterson, Natural Concentrations of Lead in Ancient Arctic and Antarctic Ice, Geochimica et Cosmochimica Acta, 45 2109-2121 (1981) (no DOE support).

C. C. Patterson[6] determined lead concentrations in sea waters off Southern California. Concentrations in surface waters were about 10 times higher than in deep waters. The rate of introduction of lead to the oceans was reported to be 27 times greater than the rate for the Pleistocene or glacial period, which indicates that the high concentrations of lead found in surface waters were caused by industrial contamination, mainly tetraethyl lead combustion products. It was concluded that biological material is the carrier for transporting lead from surface waters to sediments and that the half-life for residence time of common lead in surface waters is about 7 years.

Most recently, Patterson has become concerned with the need for studies that will disclose dysfunctions now existing within and caused by the excessive amounts of lead in most present day Americans.

He has called attention to the problem that biochemical laboratories for studying the effects of lead are as badly contaminated with lead as are people, and control animals and tissues possessing lead levels at ultra-low natural levels which could be used for comparisons with animals containing amounts of lead typical of those in most people have not been available.

Patterson has pioneered three major areas of geochemical research:

- He provided the first reliable ages of the earth and meteorites (33 years ago), utilizing elegant microchemical and precise mass spectrometric techniques for the analysis of the isotopic compositions and concentrations of lead in terrestrial materials and meteorites. His work has stood the test of time; the age of 4.55 billion years for the solar system has been confirmed subsequently by others using different techniques and materials.
- Through extensive field experimental and analytical work, he established the fundamental basis for modeling the patterns of evolution of radiogenic lead in the earth, thus creating a powerful tool for identifying, tracing and evaluating the nature of the major geochemical reservoirs in the crust, mantle, and oceans.
- He has provided the most rigorous analysis of both the natural background and the anthropogenic buildup of lead in man's environment. He did this by further extending the analytical capabilities growing out of his geochemical research and by the design and implementation of exhaustive sampling experiments in remote regions of the earth, and in ancient archeological materials. We owe to these experiments most of our present understanding of the magnitude and origins of lead pollution.

The AEC support for Professor Clair Patterson and his students originally was for geologic research aimed at exploiting the newly developed capabilities for using radioisotopes in a rather elegant experimental program to quantify geologic processes. Concern about industrial contamination of the natural lead tracers led to research identifying the extent of such contamination and the processes involved. The direct consequence of this research was the identification of the extent of airborne contamination by tetraethyl lead aerosols, efforts relating such contamination to human health concerns, recognition of the solution to the problem through immediate reduction of tetraethyl leaded gasolines, which was its principal use and the principal source of contamination.

An interesting question arises always when basic research is examined as an activity for Federal funding. It basically is a question of the economic value or payoff the Nation

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[6] M. Tatsumoto and C. C. Patterson, The Concentration of Common Lead in Sea Water, Earth Science and Meteoritics, J. Geiss and E. D. Goldberg, eds., North-Holland Publishing Co., Amsterdam (1963). [Partial AEC support for this work was acknowledged in this chapter.]

might expect from funding such work. What has been the economic benefit of eliminating leaded gasoline? We don't know, but we venture to guess the benefit if measured in terms of human health probably continues to far exceed the annual budget of the Basic Energy Sciences program, which now runs at about half a billion dollars annually.

Supersonic Transport Effect on the Ozone Layer

The Office of Basic Energy Sciences and its predecessors have for many years supported the research of Professor Harold Johnston in the general area of chemical kinetics. Professor Johnston's research interests involved the chemistry of nitrogen oxides (NO_x). The proposal in the late 1960's of a Super Sonic Transport (SST) that would fly at an altitude in the region of relatively high ozone (O_3) concentration led Professor Johnston to suggest that the NO_x emitted by the aircraft engines would affect the overall concentration and level of O_3 in the atmosphere. Without the knowledge gained through basic research on atmospheric chemistry, awareness of the potential for violating the integrity of the protective ozone layer would not have existed.

In the late 1960's, the plan to develop an aircraft capable of supersonic flight (SST) was under active consideration in the United States, the Soviet Union, and by a consortium in Great Britain and France. Plans indicated that the aircraft would fly at supersonic speeds and altitudes between 17 and 20 km, a region of the stratosphere just below the ozone concentration maximum which is at 25 km. If there were to be an impact upon the delicate ozone layer, the American aircraft would have the greatest effect since it would fly at the highest altitude and have the most powerful engine of the three models.

A university-sponsored study in 1970 on critical environmental problems expressed concern that a large fleet of SST's, estimated to be about 500 planes, might affect the stratosphere through increased cloudiness with the concomitant formation of a stratospheric smog formed from the emission of engine combustion products.[7] The chemical impact of added water vapor from the engine exhausts upon the stratosphere was also considered. Its relative importance on ozone concentrations has changed many times, from being considered important to unimportant, over the years.

It was at a conference convened for the express purpose of examining the role of chemistry on the potential modification of weather and climate by a fleet of SST's that Harold Johnston of the University of California and LBL, who was specifically invited to attend, brought up the issue of the effect of nitrogen oxides upon the ozone layer.[8] Shortly thereafter Johnston published a paper in Science[9] suggesting the significant depletion of stratospheric ozone as a possible result of SST operation. This paper concludes:

"...the purpose of this report is not to say precisely by what factor the O_3 shield will be reduced by SST operation, but rather to point out that the variable (NO_x) that has been discounted is much more

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[7] L. J. Carter, Science, 169, 600 (1970).

[8] L. Dotto and H. Schiff, The Ozone War, Doubleday and Co., New York, 1978.

[9] H.S. Johnston, Science, 173, 517 (1971) - support from the AEC is acknowledged.

important than the variable (H_2O) that has been given so much attention. Just as the ... report incorrectly discounted NO_x and the SST planners for several years overlooked the catalytic potential of NO_x, it is quite possible (and, in fact, highly probable) that I have overlooked some factors, and the effect of NO_x on the O_3 shield may turn out to be less, or greater, than that indicated here."

Johnston had identified a potential threat to the fragile ozone layer.

Professor Johnston's research interests were related to tropospheric chemistry, smog formation from nitrogen oxide automobile emissions as it relates to ozone formation, a major constituent of smog. He was not focused on either stratospheric chemistry or SST's. However, he had been studying the chemistry of nitrogen oxides since the mid-1940's, was the recognized expert in the chemistry and kinetics of these nitrogenous species, and had recently published a review article on neutral O atom chemistry.[10] The reaction of O atoms with molecular O_2 is, of course, the major source of stratospheric ozone.

Johnston arrived at Berkeley in 1957 and was supported by the AEC through the Lawrence Berkeley Laboratory since 1966. It is clear that without the depth and wealth of knowledge gained in his basic research effort, concern for the integrity of the ozone layer may have been overlooked. The 1971 paper was the genesis of high-level scientific concern for the stratospheric environment.

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10 H. Johnston, Gas Phase Kinetics of Neutral Oxygen Species, NSRDS-NBS Number 20 (1968).

Chlorofluorocarbons and the Ozone Layer

Professor F. Sherwood Rowland had been supported by the Office of Basic Energy Sciences in the area of hot-atom chemistry. Professor Rowland focused upon the photochemical production and chemical kinetics of the chlorine-38 isotope. The inert characteristics of the chlorofluorocarbons (CFC's) were well known, but Rowland, as a result of his intimate knowledge of Cl atom sources, suggested (with M. Molina) in 1974 that the addition of inert chlorofluoromethanes into the environment could have a severe effect upon the ozone layer. The compounds will remain chemically inert and will diffuse to the stratosphere where photodissociation would produce Cl atoms and trigger a chain reaction that could cause significant depletion of the ozone layer.

The presence of an O_3 "hole" in the Antarctic was published in 1985, and the article showed a 30-year period of O_3 measurements taken at the British Antarctic Survey station at Halley Bay. The data showed a drastic decrease in ozone during the spring with the effect intensifying during the 1980's. Many theories were proposed to explain the phenomena. The one that is presently accepted was proposed by Rowland as part of his Chemical Sciences-supported research. The theory invoked heterogeneous reactions on polar ice clouds of chlorine nitrate ($ClONO_2$) with HCl and H_2O to produce labile sources of Cl atoms that could then reinstitute the chain decomposition.

Professor Rowland had been supported by the AEC since 1956 in the area of hot-atom chemistry, i.e., chemistry of translationally excited species that commonly were formed as the result of nuclear reactions.

The focus of his work was on the kinetics of hot halogen atoms such as chlorine-38. As the result of his attendance at an international conference in Vienna, Rowland's interest was piqued by a then recent measurement of the atmospheric concentration of fluorocarbons.

Over the years, Rowland has introduced new subjects into his research, including photochemistry and the chemistry of fluorine, both of which laid the foundations for the fluorocarbon work that would follow. In the summer of 1973, Rowland called his sponsors at the AEC and told them he wanted to branch out -- they seemed agreeable to the idea -- to study the fluorocarbons. This was a somewhat curious request since it had nothing even remotely to do with nuclear energy. But researchers who have proven to be productive in the field of basic research are often given a relatively free hand since the benefits of such research are frequently unexpected and can neither be predicted nor planned.[9]

The inert characteristics of the chlorofluorocarbons (CFC's) were well known, but with his intimate knowledge of Cl atom sources, Rowland reasoned that though chemically inert they could be photolyzed to produce atomic chlorine by short wave ultraviolet light were they to reach the stratosphere by diffusion. The initial thoughts led to the recognition with Mario Molina that, comparable to the catalyzed destruction of O_3 by NO_x, the photolytically produced Cl atoms could also catalyze the destruction of ozone through the simple chain mechanism:

$$Cl + O_3 = ClO + O_2$$
$$ClO + O = Cl + O2$$

The net reaction is:

$O + O_3 = 2O_2$, a loss of ozone.

The work was published in Nature in 1974.[11]

In September 1986, Professor Rowland had advanced a theory, backed by modeling studies with collaborators at NCAR, for ozone depletion in the Antarctic atmosphere involving heterogeneous reactions on polar ice clouds of chlorine nitrate with HCl and H_2O. Rowland's chlorine nitrate explanation was one of many (including ClO and BrO reactions, volcanic aerosols, and a hyperactive sun) which followed in a flurry of activity by scientists from many disciplines to solve the puzzle. Recent laboratory results at simulated Antarctic conditions from two separate research groups, at the NASA Jet Propulsion Laboratory and SRI, appear to have validated the chlorine nitrate hypothesis.

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[11]M.J. Molina and F.S. Rowland, Nature, 249, 810 (1974) - support from the AEC is acknowledged.

Global Geochemical Cycles and Climate Change

This item and the next three discuss examples of current research in the Office of Basic Energy Sciences relevant to environmental concerns.

Among the research activities at the Center for Isotope Geochemistry at Lawrence Berkeley Laboratory are several studies related to the environment, notably in the areas of global geochemical cycles and climate change.

Chemical weathering of rocks removes CO_2 from the atmosphere and, thus, measuring time in scales of 10^6 years may be one of the major determinants of global climate. A study of isotopic ratios of strontium (Sr) in seawater revealed variations in the rate of global chemical weathering over the past 2.5 million years (Capa and DePaolo, 1990).

Other measurements of marine Sr isotope ratios provided evidence that increases in the global chemical weathering rate precede episodes of global climatic cooling and, therefore, may be a primary cause of such events (DePaola and Finger, in press). Results of other isotopic studies from these authors reveal a role of tectonics in controlling weathering rates and global climate.

Results of geochemical and stable isotope studies from two Deep Sea Drilling Project Sites (Staudigel et al., 1989) present a serious challenge to the Berner, Lasaga, and Garrels model of the global geochemical cycle of carbon. The seafloor weathering of oceanic crust removes considerable carbon from seawater. The calculated flux of carbon into the seafloor via this mechanism is approximately equal to the total flux of carbon from degassing at mid-ocean ridges. This work points out our limited understanding of global carbon cycles and suggests means by which we can further our understanding.

Modeling studies are in progress, designed to demonstrate methods by which isotopic measurements may be used to evaluate contaminant transport in the subsurface. In addition, the application of these models to past changes in ocean temperatures during glacial episodes is expected to improve our records in this area.

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Use of Geophysical Methods for Environmental Studies

Geophysical methods are being developed at Lawrence Berkeley Laboratory to improve our capabilities to image structure, properties and processes in the subsurface. Seismic and electrical methods are being developed, both independently and in combination. Such technology has direct application to the problems of characterizing and monitoring waste contaminated sites.

The key element that lets us detect environmental wastes is water. Ground containing waste-contaminated water can be monitored for its water content using geophysical methods. The next step is to use this result to map the contaminated zone and then characterize it based on information obtained from laboratory experiments. Under favorable conditions, by continuously monitoring over a period of time, we could even describe the apparent flow in such a contaminated zone.

The electrical conductivity of rocks is controlled by the fluids and their conductivity. Fluid saturation, in particular, has a dramatic effect on the conductivity of rocks. As water is withdrawn from a saturated rock the large pores empty first, but the bulk resistivity increases slowly since it is mainly controlled by the small water passageways. At this point the rock resistivity is roughly proportional to the inverse of saturation squared. As desaturation progresses, a critical saturation is reached at which point there is no longer any water to conduct along some pores. This breaking of the conduction paths leads to a much more rapid increase in resistivity, roughly proportional to one over saturation to the fourth power. The critical saturation depends on the rock type (the nature of the porosity) and may depend strongly on the role of the fractures that may be present.

Experimental data show an opposite phenomena in the seismic velocity. There is a slow but gradual change in the velocity when the rock is only partially saturated. As the rock gets nearly fully saturated, the velocity increases dramatically. This is encouraging because the saturation affects the resulting electrical conductivity and seismic velocity in different ways and, therefore, these two methods can be used in a highly complementary manner. Furthermore, one method may provide an excellent structural picture of the rock unit contaminated by the wastes while the other may detail the variation of rock properties within the same unit.

With the advancement of medical tomography, applications of tomography to geophysical imaging problems, including transmission and diffraction tomography using seismic and radar-frequency EM data, have followed. Due to the limitation of short penetration depth (at most a few meters) inherent in radar applications, a technique called diffusion tomography (Zhou, 1989) has recently been developed at LBL for analyzing crosshole audio-frequency EM data. The frequencies needed depend on the overall size of the structure, but typically are in the range of a few kHz to tens of kHz. Wave field diffraction tomography involves Fourier transformation of the data, filtering of the transformed data, back propagation, and eventual inverse Fourier transformation to construct the image. This simple procedure cannot be applied to the diffusion tomography. Instead, a system of linear equations was constructed to obtain the discretized object function (image). To test the numerical technique, a simple 2-D case has been considered. The model was two thin conductors simulating parallel fracture zones embedded in an otherwise uniform whole space of 0.01 S/m. A line source carrying an ac current of frequency 10 kHz was used to excite the medium. Using a 2-D forward modeling algorithm, a set of data was generated corresponding to a total of 32 sources and 32 receivers. Using this synthetic data set, an image was successfully reconstructed with a good resolution. To provide real data sets for the testing of such numerical algorithms, however: (1) an EM scale-model experiment is being conducted; and (2) a small-scale field experiment is underway at the Richmond Field Station (RFS), University of California.

1. ***Scale Model Study*** -- The scale model consists of a container of size 9' x 15' x 4' filled with 10 S/m saltwater. Graphite blocks are used as targets and an array of transmitter and receiver coils are used to measure the resulting magnetic fields. The system has been designed such that data is collected at a fixed position while the transmitter moves continuously. This provides for both low noise measurements and relatively quick acquisition. The system has been verified to be working by three independent tests. Tests have shown the repeatability to be better than 1% of the primary field over the period of 1 day. Data sets collected for receiver depths of 0, 10, and 50 cm in the absence of the graphite block have been inverted using one-dimensional (1-D) code, and the result shows the air-saltwater-concrete sequence with correct electrical resistivities.

   Lastly, measurements made at the same receiver positions in the presence of a graphite block have been compared to computer-generated numerical solutions, and the agreement is excellent.

Currently, a large data set consisting of measurements made at 45 receiver locations at intervals of 2.5 cm is being collected. This data will be used to image the graphite block using the diffusion tomography algorithm developed by Zhou (1989). The same data set will be used to test the inversion algorithm developed by Eaton (1987) and Eaton and Hohmann (1988).

2. ***Field Test*** -- In a small-scale field experiment at the RFS, more than 20,000 gallons of seawater will be injected into a shallow underground aquifer and the associated change in subsurface conductivity will be monitored with EM measurements in boreholes spaced 50 meters apart, straddling the injection well. The crosshole EM system consists of a borehole transmitter, which broadcasts sinusoidal signals at frequencies 5 to 10 kHz, and a computer controlled receiver section. The receiver consists of a bore-hole probe connected to a lock-in amplifier, all controlled with a desktop computer.

The crosshole survey will utilize multiple transmitter and receiver positions for a total of more than 400 separate measurements. A complete set of data will be collected before injection begins and daily during the saltwater injection and withdrawal.

References:

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Eaton, P.A., 1987, Three-Dimensional Electromagnetic Inversion: Ph.D. Thesis, University of Utah.

Eaton, P.A., and Hohmann, G.W., 1988, Three-Dimensional Electromagnetic Inversion: Expanded Abstracts, 58th Annual International SEG Meeting.

Use of Robots to Clean Nuclear and Chemical Wastes

The Engineering Program of the Office of Basic Energy Sciences supported the establishment of the Center for Engineering Systems Advanced Research (CESAR) during FY 1984 at the Oak Ridge National Laboratory (ORNL) for the purpose of addressing fundamental research and issues associated with the development of intelligent robotic machines so as to help increase productivity and safety in the design and operations of DOE-sponsored systems and programs. One aspect of the program at CESAR has consisted of the development of an evolving series of mobile robot prototypes called HERMIES (Hostile Environment Robotic Machine Intelligence Experiment Series). These robots are used to test new methods, to develop hardware and software, and to evaluate the performance of various robotic system components in integrated systems. Currently operational are the mobile robots HERMIES-IIB and III.

Because of the excellent performance record of CESAR in bridging the gap between basic research and demonstration, testing, and evaluation of robotic systems, it has attracted the attention from other offices within DOE and from many non-DOE sponsors. For example, CESAR is now a contributor to the National Robotics Technology Development Program for the Office of Environmental Restoration and Waste Management.

The basic research and development has been translated into high levels of performance. Recently, experiments with HERMIES robots have demonstrated their ability to navigate in an incompletely known, dynamically changing laboratory environment with unexpected events, to perform diagnosis, learning and simple manipulation tasks at a mock-up process control panel, and to remove a simulated chemical spill in the laboratory. HERMIES-IIB has been used in experiments showing capabilities in world modeling, autonomous navigation in dynamic experiments, handling of contingencies, sensor-guided exploration and goal recognition. robot vision, vision guided manipulation, and innovative problem-solving based on prior experience.

In the most recent experimental setup, HERMIES-III was used to demonstrate the capability of a robot to cleanup a simulated chemical spill. The approximate location of the chemical spill and instructions to clean up the spill were programmed into the robot. A vacuum attachment to the end-effector on the manipulator arm was adequate to clean the material (coffee ground or liquid substances) used to simulate the spill. Based on only partially complete geometric information about the robot's environment, HERMIES-III was able to plan a path and navigate, avoiding obstacles along the way, to the presumed location of the spill. Using its vision system, the robotic machine determined the extent and precise location of the spill and calculated and executed a motion pattern for the seven-degree-of-freedom manipulator arm to effect the removal of the spill. This experiment was made possible by the integration of a number of system modules and associated processes which were executed simultaneously and asynchronously on a network of several computer systems.

The ongoing research program supports the continued development of autonomous capability for HERMIES-IIB and III to perform complex navigation and manipulation under time constraints, while dealing with imprecise sensory information. Detailed descriptions of the research on robotic systems at CESAR can be found in more than 130 publications.
Dr. Reinhold Mann is the current Director of CESAR.

Underground Imaging and Borehole Technology

Since the late 1970's, BES has supported development of technology for underground imaging. These technologies are geophysical applications of tomography, developed to yield high resolution images of underground structure and processes. The first geophysical tomograph of underground structure was made in 1975 by scientists from Lawrence Livermore National Laboratory. It was an electromagnetic attenuation image of a coal seam in Kemmerer, WY. Since that time, the art and science of geophysical tomography have matured significantly. Field-worthy automated data systems have been built and used extensively by government and industry; acoustic, electromagnetic and electrical energy has been used to generate images; recent computational advances have made practical real-time data reduction and image processing; new, sophisticated and efficient algorithms have been developed for image reconstruction. Since those early days, a wide variety of problems have been addressed with underground tomography. These include <u>in situ</u> oil shale process monitoring, fracture characterization, location of tunnels and voids, hydrology studies, oil field characterization, and steam and fire flood monitoring for enhanced oil recovery.

Underground imaging technology is also used for characterizing and monitoring clean up of hazardous waste sites. For example, two environmental projects have recently been started at the Lawrence Livermore National Laboratory. One is an effort to understand the transport of contaminants from the surface to the water table through the intervening, complex, inhomogeneous soil. High resolution images are being made as a function of time as the contaminant-carrying plume develops from the surface and progresses through interbeds of gravels, sands and clays. The second is an effort to monitor an experimental cleanup at a DOE facility of a trichloroethylene ground water plume. Images are being made to determine the response of the water table as air is injected underground to effect an air stripping of the contaminant.

In order to determine the scientific feasibility of extracting energy directly from magma, the BES Geosciences program supported the development of a downhole seismic signal generator at the Sandia National Laboratories in Albuquerque, NM. That tool is now being used at Savannah River to monitor their steam strip cleanup and interest has also been expressed in its use for characterizing waste sites and cleanup areas. The tool has also been used by the petroleum industry for enhanced oil recovery and the technology is being transferred to industry. Under the same effort, a directional flow tool is now being used in conjunction with the City of Albuquerque Hydrology Department to monitor groundwater flows and in the Savannah River cleanup to monitor groundwater flow during remediation. This system is also in the process of being transferred to industry.

Subprograms

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

Materials Sciences

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

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

Examples of research accomplishments this past year include:

1. ***High-T_c Superconductor Wire Fabrication Technology*** -- At Argonne National Laboratory (ANL) technology was developed for coating metal wires with malleable precursor elements of the high T_c superconductors that contain the rare-earth metal yttrium. When these wires are heated, the elements form the less malleable high T_c superconducting ceramic around the wires. These composites, thus, provide the mechanism for the fabrication of wires sufficiently long and strong for high T_c superconductor applications. A private company formed in 1988 to commercialize new superconductors agreed in 1989 to license this technology from Argonne and to provide $100,000 to ANL for research on other superconductor technologies.

2. ***New Process for Synthesis of Silicon Carbide*** -- A new, simple, efficient route to the synthesis of silicon carbide was developed at Ames Laboratory in 1989 accompanied by development of a process to produce the silicon carbide in the form of fibers. This process involves surface crosslinking of silylene-acetylene (Si_2H_2-C_2H_2) polymer fibers allowing the fiber structure to be maintained throughout the process of pyrolytic conversion of the polymer to silicon carbide. The industrial fabrication of silicon carbide fibers has been a technological secret closely guarded by the Japanese, and this result has been viewed as a major breakthrough. By adapting this new technology to a continuous process, the cost and production time of current commercial (Japanese) routes to silicon carbide fibers could be cut. These fibers are used in composites which are displacing metals in industrial applications due to their high strength, low weight, high heat tolerance, and resistance to chemical breakdown.

3. ***Calculations of the Heat of Formation of Alloys*** -- Many materials with excellent strength or high temperature properties are alloys. The number of possible alloy combinations is very large and theoretical guidance for choosing promising alloys to investigate is of great interest. In recent years, it has become possible to calculate, from fundamental theory, the energy or heat released when two metals form an alloy. This theory was applied to 24 alloys typified by titanium-platinum; the calculations successfully predicted the crystal structure for 50/50 and for other alloy compositions as well as the high heats of formation found experimentally. Calculations of the type made are not limited to the metals studied in this work, and unknown alloy properties were found to be predictable. In 1989, the technologically important material, nickel aluminum, was investigated. Calculations of this type are expected to be extremely helpful in the search for new alloys.

4. ***New Ion Conducting Polymers*** -- A new class of silicon-based ion conducting polymers with the highest room-temperature conductivity ever measured for such materials was developed. Room-temperature conductivity was 10 times higher than for any other polymeric material. This development is expected to have an important impact on thin film electrochemical energy technologies, particularly rechargeable lithium batteries and electrochromic windows. Thin film rechargeable lithium batteries based on solid polymer electrolytes, lithium anodes, and lithium materials as cathodes have theoretical energy storage capacities more than 10 times that of lead-acid or nickel-cadmium batteries. This class of materials is attractive for long-term energy storage because self-discharge rates for lithium batteries have been below 0.1 percent per year, implying a shelf-life of more than 10 years.

5. ***Biological Process Grows Oriented Ceramic Crystal*** -- A new method for growing oriented ceramic thin films was developed. It mimics natural biological processes that produce seashells, bone, tooth enamel, etc., to grow oriented thin films of a desired ceramic material. This process is unique; it uses a surface-modified polymer as a template to control crystal orientation and size as the crystals grow from a solution. Crystal growth occurs only where the polymer has been modified; thus oriented growth is easily achieved by selective polymer surface modification. The process takes place near room temperature and essentially controls the placement and orientation of each ceramic crystal. Oriented films as thin as 200 A and as thick as several microns have been grown. This process offers a method of combining polymers and ceramics into unique monolithic composite materials (by layering) which have high resistance to brittle failure. An entirely new class of ceramic matrix composite materials can now be fabricated with only a few percent polymer that controls crystal orientation and greatly influences fracture toughness of the material.

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

1. ***Lattice "Stiffening" Observed During Superconducting Transition*** -- The first direct evidence of an abrupt "stiffening" of the crystal lattice at the superconducting transition temperature was obtained using the unique technique of ion channeling. The measurements, performed on highly perfect single crystals of

$YBa_2Cu_3O_{7-x}$, involved steering an ion beam along the channels between atomic rows and planes of the single crystal. The scattering of the individual ions within the channels provided a direct probe of the vibrational amplitudes and, hence, lattice stiffness. This was the first direct evidence of a step-wise increase in lattice stiffness at the superconducting transition temperature. Structural information, also obtained by the channeling technique, confirms that no crystallographic transformation occurs at the transition temperature.

2. ***High Temperature Superconductors*** -- The fundamental properties of yttrium-based and thallium-based superconductors were studied yielding some new insights into the relationship between these properties and processing conditions. Processing studies of $YBa_2Cu_3O_{7-x}$ used in situ Raman spectroscopy to determine the relationship between oxygen defects (deviation from a perfect crystal structure), temperature, and superconducting transition temperature. A phase transition involving the oxygen displacement within the structure was observed for the first time. In a collaborative study, substituting oxygen at selective sites in $YBa_2Cu_3O_{7-x}$ was used to determine the distribution of oxygen isotopes at different sites within the structure. Fundamental characterization of four different thallium-based superconductors was performed using polarization studies of oriented single crystals. This information was used to characterize the spatial distribution of phases within polycrystals. By Raman microscopy, it was found that the majority of thallium-based crystals had intergrowths of several phases within them.

3. ***Observation of Phonon Coupling in a High T_c Superconductor*** -- Careful measurements on the $Ba_xK_{1-x}BiO_3$ system [superconducting transition temperature (T_c) of 30K] permitted the unequivocal determination of an isotope effect on T_c showing a major role for phonon coupling (electron-lattice vibration interactions) in a high-temperature superconductor. This work was made possible by the development of a unique, simplified method for synthesis of the compounds used. With good samples available, a large number of pertinent basic properties, including structural phase relationships, normal-state resistivity, superconducting energy gap, and critical fields were measured, making $Ba_xK_{1-x}BiO_3$ one of the most completely characterized oxide superconductors available. Understanding the role of phonon coupling allows the development of realistic models to help predict additional technologically important properties of the system, such as critical current. Since the structure of this superconductor is cubic, it is easier to theoretically model its properties and use the results to evaluate the role of phonon coupling in other compounds to gain a better understanding of the ultimate T_c in the oxide superconductors generally.

4. ***$KTaO_3$ - A New Substrate Material for High-T_c Superconducting Films*** -- A new crystalline substrate for the formation of thin films of high-T_c superconductors was discovered. The new material, potassium tantalate or $KTaO_3$, can be used to grow thin, aligned crystalline films of the $YBa_2Cu_3O_{7-x}$ family of high-temperature superconductors. Substrate materials for the growth of thin films must meet a set of stringent requirements, including a close match between the lattice constants of the film and substrate and a high degree of chemical inertness to prevent film-substrate reactions that destroy the superconducting properties of the film. The new materials meet both of these critical criteria. In fact, the $KTaO_3/YBa_2Cu_3O_{7-x}$ system is apparently characterized by a lower degree of substrate/film interaction

than that associated with any previously employed substrate material such as $SrTiO_3$. Fortunately, the new substrate material can be grown in the form of large single crystals relatively simply so that it is a practical material for production of large-scale electronic devices.

With support at an operating level of $197,072,000 in FY 1990, Materials Sciences provides more than one-third of the total Federal funding for basic materials research.

The Materials Sciences subprogram emphasizes selected areas of fundamental importance and areas where critical problems have emerged 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., high-temperature superconductivity), and still other research has more fundamental implications underpinning all materials research, e.g., mechanisms of electron, atom or ion transport in solids or computer modeling of materials phenomena. This subprogram is the basic research activity in DOE underpinning materials development efforts for all the energy technologies. 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.

Besides maintaining an appropriate mix of long-term scientific, multi-technology, 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 pursuing its research goals. These facilities include the National Synchrotron Light Source (NSLS) and the High Flux Beam Reactor (HFBR), both at Brookhaven National Laboratory; the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory; the Manuel Lujan, Jr. Neutron Scattering Center, LANSCE, at Los Alamos National Laboratory; the Advanced Light Source (ALS) under construction at Lawrence Berkeley Laboratory; the Advanced Photon Source (APS) under construction at Argonne National Laboratory; and the electron microscopy facilities at Oak Ridge, Argonne, and Lawrence Berkeley Laboratories.

Operation of these facilities took about 31% of the FY 1990 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.

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 Division of Materials Sciences' Council on Materials Science (a body with representatives from academia, industry, and agency laboratories) help to focus attention on critical issues. Three recent panel studies were held on Fundamental Issues in Heteroepitaxy, Surface Interface and Thin-Film Magnetism, and Clusters and Cluster Assembled Materials. The Department 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 Office of Energy Storage and Distribution and the Division of Chemical Sciences entitled The Role of Interfaces in Metal-Air Battery Electrochemical Reactions.

Current emphases and trends include high-temperature superconductivity, 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 subprogram can be obtained from I. L. Thomas, Director, Division of Materials Sciences, ER-13, Office of Basic Energy Sciences, Department of Energy, Washington, D.C. 20585, (301) 353-3427.

A detailed summary of current projects is published annually. The most recent (September 1989) is entitled "Materials Sciences Programs, Fiscal Year 1989" (DOE/ER-0447P).

Chemical Sciences

The Chemical Sciences subprogram sponsors experimental and theoretical research on liquids, gases, plasmas, and solids. The focus is on their chemical properties and the interactions of their component molecules, atoms, ions, and electrons. The subprogram objective is to expand, through support of basic research, our knowledge in the various areas of chemistry; the long-term goal is to contribute to new or improved processes for developing and using domestic energy resources. At a budget level of $140,256,000 in Fiscal Year 1990, this subprogram is a major source of Federal support for basic chemical research in the United States. Disciplinary areas covered include physical, organic, and inorganic chemistry; chemical physics; atomic physics; photochemistry; radiation chemistry; thermodynamics; thermophysics; and analytical chemistry.

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

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

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

Examples of research accomplishments this past year include:

1. ***Supercritical Fluid Expansion Process Produces Uniform Particles for Thin Films and Fibers*** -- A new method was developed for the formation, directly from a vapor, of chemically and physically uniform submicron particles of many materials. The process uses supercritical fluids as solvents for the material to be deposited. The solution is

rapidly expanded through a small nozzle from a supercritical fluid state into a volume where the solvent changes to a low pressure gas. The material thus released from solution forms fine particles that can be collected on a surface. The process lends itself to the formation of thin films and fibers and uniform mixtures of substances that cannot ordinarily be combined. Because many supercritical fluids form at room temperature, heat sensitive materials like biological molecules and organic polymers can be processed by this method. This new process is a spinoff from earlier research supported by BES and has been awarded several patents and received an R&D 100 Award in 1988.

2. ***Reaction Rate Data Confirm the Role of Quantum Mechanical Tunneling in Chemical Reactions*** -- Scientists at Argonne National Laboratory and the University of Illinois at Chicago, in separate but complementary studies, have confirmed the role of quantum mechanical tunneling in the reaction of oxygen atoms with hydrogen molecules to yield the chemical radical OH and a hydrogen atom as products. The effect of quantum mechanical tunneling is to allow chemical reactions to take place when the combined energy of the reacting species is insufficient to break the chemical bonds of the reactants, in this case the H_2 bond. Knowledge of the influence of tunneling is necessary to extrapolate chemical reaction rates from temperatures and pressures characteristic of laboratory measurements to conditions characteristic of combustion processes. Because hydrogen is the lightest element, it is expected to exhibit the largest quantum mechanical tunneling effect. Earlier measurements of $H_2 + O$ and $HD + O$ reported last year had indicated that tunneling might, indeed, have a significant influence on the temperature dependence of the reaction rate. The recent measurement of $D_2 + O$ now confirms the earlier measurements. The data have been compared with theoretical predictions from Argonne, the University of Minnesota, and Emory University, all of which were supported by the DOE Office of Basic Energy Sciences. Agreement between both sets of measurements and theoretical calculations was excellent. The theory and data will be useful in placing limits on the influence of tunneling in other chemical reactions.

3. ***Spectral Hole Burning: a New Window on Photosynthesis*** -- A spectroscopic technique known as "spectral hole burning" has provided an unprecedented level of detail in the study of electronic excitations that take place in photosynthetic reaction center and light harvesting complexes. In studies of purple bacteria, it was shown that the "special pair" of chlorophyll molecules in the reaction center undergoes a slight geometrical rearrangement upon the light excitation that induces the separation of positive and negative charges. This rearrangement cannot be observed by X-ray diffraction which records the structure of the reaction center when it is not excited. The ultra-short time required for charge separation, 1 picosecond, was also determined from the hole burning measurements. In light harvesting complexes of green plants, new information has been obtained on the mode of energy transfer from the antenna chlorophylls to the special pair in the reaction center. The hole burning technique, developed by Dr. Small, has led to improvements in spectral resolution from two to four orders of magnitude, thereby turning quite featureless spectra into spectra rich with structure.

4. ***Surprising Molecular Rearrangement Seen in Molecular Beam Studies*** -- Molecular beam studies of the photodissociation of benzene have produced some surprising results. In the experiment, benzene, a ubiquitous but minor constituent of hydrocarbon

fuels and a precursor of soot in combustion, was exposed to ultraviolet laser irradiation exciting the benzene to a dissociative state. The surprising result was the appearance of the methyl radical, CH_3, among the dissociation products. The reason this is surprising is the extensive migration of hydrogen atoms necessary to produce CH_3. Benzene consists of six carbon atoms in a ring with a single hydrogen atom bonded to each carbon. The expected products from the dissociation of benzene would thus be C_2H_2 or C_3H_3. CH_3 requires the migration of two additional hydrogen atoms to one of the carbon atoms in the molecule before the ring fragments. This is very likely the most extensive intramolecular rearrangement ever seen for a simple molecule, is currently unexplained, and has significant implications for chemistry where most chemical reactions are expected to proceed via simple, single-step bond breaking and formation.

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

About one-third of the Chemical Sciences operating budget for FY 1990 supports facility operations and nearly 30% directly supports research at universities. At the DOE laboratories, interactions between basic researchers and research and development teams working in energy technology areas are encouraged. National laboratory scientists, 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.

Coordination between basic researchers supported by Chemical Sciences and the scientists in the energy technology programs and industry is encouraged. Various conferences and committees, e.g., the Solar Photochemistry Research Conferences, Catalysis Research Meetings, and the Hydrogen Energy Coordinating Committee, identify research needs and opportunities, compare results, and coordinate activities within DOE and with the rest of the scientific community. Reports such as the National Academy of Sciences/National Research Council's Opportunities in Chemistry and DOE's Energy Research Advisory Board review of it, 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.

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

Applied Mathematical Sciences

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

Scientific advances traditionally have depended on experiments for data and on theory for understanding. Today there exists a third and equally important component of scientific research: computational science. Computational science is both an experimental tool and a tool for extending theoretical understanding and interpretation of experimental data. 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 has been brought about by our increasing ability to do computational modeling of physical problems and by the enormous power of the modern supercomputer. This combination allows scientists and engineers to model complex problems realistically and to obtain more accurate answers than were possible a few years ago.

The primary objective of the Mathematical Sciences Research activity is to advance our understanding of the fundamental concepts of mathematics, statistics, and computer science. These concepts underlie the complex mathematical models of key physical processes encountered in the research and development programs of DOE. This activity also supports investigations of advanced computer architectures that may lead to new approaches to supercomputers.

Three major categories of Mathematical Sciences Research are supported at the national laboratories, universities, and at private research institutions: Analytical and Numerical Methods, Information Analysis Techniques, and Advanced Computing Concepts, the emphasis in each case being on new parallel-multiprocessor architectures. This activity also established several experimental computing research facilities to support the exploration of new concepts in large-scale scientific computing.

The projects supported have two important facets that require substantial cooperation and coordination among traditionally separate groups. One facet concerns interdisciplinary teams of computational scientists, computer scientists, and mathematicians working together on all aspects of large-scale scientific computing problems. The other facet involves the cooperation of industry, government, and universities on the design and implementation of prototypes of several potentially strong candidate architectures; this facet is 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 should benefit from these cooperative projects through improved understanding gained of architecture and software trends and issues that currently tend to limit the industrial use of supercomputers today. 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 is being coordinated with programs of other agencies to share facilities wherever possible.

The Energy Sciences Advanced Computation activity provides scientific supercomputer access required by researchers in the Energy Research programs except for Fusion Energy. Beginning in 1985, the use of the Energy Research Supercomputer Center (NERSC), formerly the Magnetic Fusion Energy Computational Center, and its network were expanded to researchers supported by the following DOE/ER programs: High Energy and Nuclear Physics, Basic Energy Sciences, Health and Environmental Research, and the Superconducting Super Collider. This center now operates a CRAY X-MP (two processors and 2 million words of memory), the serial #1 CRAY-2 (four processors with 62 million words of memory), a CRAY-2 (four processors and 128 million words of memory) and the unique eight-processor CRAY-2 (128 million words of memory). The NERSC Common File System has a capacity of more than three Terabytes (million million bytes) of tape storage. The Supercomputing Computations Research Institute at Florida State University (FSU), initiated at the direction of Congress in 1985, now operates a CRAY Y-MP (four processors with 32 million words of memory), associated Solid State Disk (128 million words), and more than 24 billion bytes of mass storage. FSU also has a 65,536 node Connection Machine (CM-2) with 2 billion bytes of central memory and a 2,000 64-bit floating point processors.

Access to these systems is provided through the Energy Sciences Network (ESNet), a nationwide data communications computer network with international connections to Europe and Japan. The ESNet is managed and funded by the ESAC activity to facilitate remote access to major Energy Research (ER) scientific facilities, to provide needed information exchange and dissemination among scientific collaborators throughout all ER programs, and to provide widespread access to existing ER supercomputer facilities. The ESNet is a 19 node backbone network which operates at T1 speed, i.e., 1.54 million bytes per second.

Examples of research accomplishments this past year include:

1. ***Time Stepping Algorithm for Parallel Computers Provides Multiplicative Speedups*** -- Parabolic and hyperbolic differential equations are often solved numerically by time stepping algorithms, which are usually regarded as sequential in time, i.e., the solution on a time level must be known before the computation of the solution at subsequent time levels can start. During 1989 it was demonstrated that it is possible for processors to perform useful work on many time levels simultaneously. Specifically, it is possible for processors assigned to "later" time levels to compute a very good initial guess for the solution based on partial solutions from previous time levels, thus reducing the time required for solution. Under this project, the theoretical and numerical implementation was developed for an algorithm that combines both parallel iterations in time as well as space, allowing computation on many time levels simultaneously. Although the time iterations initially are further from convergence, the effective number of iterations to convergence is much smaller, providing speedup factors that multiply any parallelism achieved in space variables.

2. ***A New Technique for Calculating the Properties of Atoms and Molecules*** -- With a computer big enough and fast enough, any property of any atom or molecule can be calculated from first principles. To date, no computer has been built that can treat any but the simplest of

atoms and molecules with an accuracy approaching that achievable by direct measurements. Thus, current research in quantum chemistry is aimed at finding approximations of known accuracy appropriate to specific atomic and molecular properties. One of the most helpful approximations is the separation of the effects of the outer, valence electrons which are responsible for most of the chemical properties of atoms and molecules, from those of the inner, core electrons. Heretofore, the effects of the core electron have been only approximated in most practical calculations. During 1988, scientists at the Lawrence Berkeley Laboratory found a new approach for including the core electrons much more accurately without a corresponding, prohibitively expensive increase in computational time. The approach treats the core electrons and valence electrons separately by establishing different time and energy scales for sampling the two sets of electrons. This approach has been applied to the calculation of the ionization potentials and electron affinities of Carbon, Silicon, and Germanium with encouraging results. These properties agree with experimental values to within 2% while at the same time their calculation achieves a factor of 5000 decrease in computer time when compared to a traditional calculation. Using these advances and the Department's supercomputers will put many important chemical systems within reach of theoretical calculation.

3. **Prediction of New Low Compressibility Solids** -- New materials which are harder than diamond were predicted using an empirical model and ab initio calculation of the bulk compressibility of covalent solids. It may be possible to synthesize these novel materials in the laboratory. The empirical model indicated that hypothetical covalent solids formed between carbon and nitrogen are good candidates for extremely hard materials. A prototype carbon-nitrogen system was chosen, a form based on the complex beta-Si_3N_4 structure, and a calculation of the total energy was made on the Department's Cray supercomputers at the National Magnetic Fusion Computer Center. The calculations were consistent with the model and show the new material to have a bulk compressibility equal to or less than that of diamond.

4. ***New Form of Carbon Dioxide Discovered Using Supercomputers*** -- During 1988, a new stable form of carbon dioxide was discovered using a Cray supercomputer. The discovery was made by using an ab initio, quantum chemical calculation. In such calculations, properties such as structures and internal energies are determined for atoms and molecules using only the knowledge of the charges and masses of the constituent nuclei and atoms. Because carbon dioxide involves many particles, 44 electrons and 3 nuclei, many simplifying assumptions had to be made in past calculations. With the availability of very powerful and fast computers, it is now possible to perform quantum chemical calculations for small molecules with very few simplifying assumptions. The calculation identified a second structure for carbon dioxide, a triangle in which each atom is bonded to the other two. In the familiar form of carbon dioxide, the structure is O=C=O. Although the new form is chemically unstable relative to O=C=O, its existence has practical implications in combustion chemistry where the density of available energy states is a critical role in determining chemical reaction rates. A large body of experimental data on the excited energy states of carbon dioxide exists, but a second form was not suspected. Even with the large amount of computer time (nearly 600 hours) required for this calculation, all possible configurations of the three atoms in carbon dioxide could not be considered. Even so, the calculation

which showed the new form also hinted that a third form, COO, also might exist.

More information on this sub-program can be obtained from John Cavallini, Acting Director, Scientific Computing Staff, ER-7, Office of Energy Research, Department of Energy, Washing-ton, D.C. 20585, (301) 353- 5800. A detailed summary of current projects is published annually. The most recent is entitled "Summaries of the FY 1989 Applied Mathematical Sciences Research Program", DOE/ER-0422, September 1989.

Engineering and Geosciences

The Engineering and Geo-sciences subprogram conducts fundamental research for DOE in these fields. The broader aspects of program design and emphasis are established through extensive interaction with the scientific and techno-logical communities in the fields of interest, utilizing studies by the Basic Energy Sciences Advisory Committee, the Department's Advisory Board, panels of the National Academy of Sciences, specially convened workshops, and individual interactions with scientists and engineers from universities, Federal labora-tories, industry, and related Federal programs.

Engineering Research

The Engineering Research ob-jectives are: (1) to improve and advance our knowledge of processes underlying current engineering practice; and (2) to expand the technical data base and understanding of funda-mental engineering concepts. It is the goal of the Engineering Research activity to improve our capability for anticipating and solving engineering pro-blems in energy technologies. Fundamental research is supported in both traditional engineering disciplines and interdisciplinary areas concerned especially with analysis, control, and im-provement of systems for transport of heat and fluids, and for materials processing. At present, three disciplinary areas are receiving high priority:

- *Mechanical Sciences* -- including fluid mechanics, heat transfer, and structures;
- *Systems and Control Sciences* -- including sys-tems analysis and control, and instrumentation; and
- *Engineering Analysis* -- including engineering data collection and compilation, and analysis of non-linear and non-equilibrium systems.

While Engineering Research activities are aimed at long-term goals, important appli-cations sometimes emerge surprisingly early. Several immediately applicable accom-plishments recently have included: 1) creation of new illumination technologies based on developments in high collection non-imaging optics which are leading to energy efficient applications such as compact high intensity solar concentrators, solar-driven lasers for satellite communi-cation systems, low power high intensity light emitting diodes, and improved energy efficient illumination systems; 2) pro-gress in understanding the stability of two-phase immiscible fluid motions leading to the consideration of energy efficient lubricated pipelines for the transport of slurries and heavy crude oils based upon the finding that under certain conditions the less viscous component arranges itself as a sheath at the wall, thereby allowing the more viscous phase to flow more efficiently in the interiors; and 3) new understandings of the fracture mechanics of solids and of crushing processes are leading to creative, energy reducing configurations in the pulverization of coal, ores, and other minerals whereby fine particles will be promptly removed, thereby reducing the overall grinding energy requirements.

Some other recent accomplishments in the Engineering Research area have included:

1. ***Method for Eliminating Backlash*** -- An example of an important engineering research activity underway is work which is leading to the development of redundant-drive backlash-free robotic arms. Backlash is a persistent problem in most industrial robot manipulators which employ gear trains for power transmission and torque amplification. The backlash arises from the clearances needed to allow for size and shape variations during manufacturing and for thermal expansion.

   Present techniques for reducing backlash such as precise gears, spring-loaded split-gear assemblies, and precise mechanical adjustments do not completely eliminate backlash. Recently, an investigator in the Engineering Research Program developed an innovative concept for the control of backlash in geared robotic systems. This concept utilizes a redundant unidirectional driver to assure positive coupling of gear meshes at all times, thereby eliminating the backlash. This improves the positioning accuracy and controllability of a manipulator and reduces the noise and vibration associated with gear trains. The result is a high precision, light weight, low cost, high performance manipulator. The redundantly robotic arm has a fail-safe advantage in that, except for loss of backlash control, it can continue to function when one of its driving motors fails. A patent has been applied for. A variety of additional applications appear likely outside of the field of robotics.

2. ***Improved Understanding of Water Condensation Dynamics*** -- Droplet formation occurs in expanding gas flows found in numerous natural and technological processes such as cloud formation, combustion, and steam turbine expansions. Research at Physical Sciences, Inc., supported by the Engineering Research Program, is providing a new view of how rapidly cooled vapor mixtures condense to form small droplets. As moist air expands, the gas initially behaves as if it were dry. When the gas is cooled sufficiently, however, the temperature and pressure of the moist air begin to increase noticeably from the dry air values due to heat released by the condensing water vapor. In the conventional picture of the onset of condensation, the water vapor abruptly and rapidly forms a dense cloud of very tiny droplets or clusters containing roughly 20 water molecules each. These tiny droplets then grow rapidly in the supersaturated environment while the total number of droplets remains essentially constant.

   Recent condensation experiments in an expansion nozzle and theoretical calculations have shown that a rather different sequence of events actually occurs. The experiments rely on scattered laser light to probe the number and size of the water droplets throughout the entire condensation zone, providing a level of detail previously unavailable. The first droplets detected by the laser are surprisingly large, containing tens to hundreds of thousands of water molecules, only a short distance after the apparent onset of condensation. The number of droplets does initially increase quickly, but then, contrary to conventional expectations, the number decreases rapidly before leveling off. The most reasonable explanation of these observations is that many droplets spanning a wide range of sizes must be present at onset. The largest, most stable droplets grow quickly at the expense of the unstable and rapidly evaporating, smallest droplets. Calculations of the number of droplets of each size present at each point in the flowing gas confirm this new interpretation and reveal details of the condensation process inaccessible to experimental observation.

First, contrary to the notion that condensation in a nozzle is triggered by the rapid formation of very small clusters, the calculations show that, at the apparent onset of condensation, the largest droplets with tens to hundreds of thousands of molecules are already substantially more abundant than the smallest clusters. Furthermore, the amount of mass contained in these large droplets far exceeds that found in the smaller sizes: it is the presence of these large clusters that is responsible for the heat released in the gas. These large clusters began forming gradually well upstream of the observable onset of condensation, and it is the rapid growth of those large droplets, and not the formation of large numbers of the tiniest droplets, that produces the visible consequences in the flow. In effect, condensation is already well underway before the apparent onset point.

The presence of surprisingly large particles early in an expansion could be a significant consideration in designing expansion processes to either enhance or avoid particle formation. The improved understanding of particle formation resulting from the work should be important for many applications including, for example, aerosol formation, wind tunnel and turbine design, exhaust plume formation, and material processing technologies using cluster beams. It may also affect our view of the formation of clouds and related studies of climate changes.

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 teleoperation applications for handling radioactive materials. The CESAR program is building on that experience in performing research on intelligent machines, i.e., man-made 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 in the mid to late 1980's 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, provides guidance for this four-part research program. Personnel exchanges, including graduate students, have been a feature of this collaboration and other universities are now participating in this venture.

Geosciences

The objective of the Geosciences activity is to develop a quantitative understanding of the energy-related aspects of geological processes. The primary focus is on the geophysics and geochemistry of rock-fluid systems. Topics emphasized include high resolution underground imaging, isotopic studies, and hydrocarbon-bearing sedimentary formations.

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; and

- *Solar-Terrestrial/Atmospheric Interactions.*

During the summers of 1989 and 1990, teams of scientists from the U.S. Geological Survey (USGS), DOE, and several universities undertook detailed in situ studies in the vicinity of the Novarupta Vent of the great Katmai eruption of 1912 on the Alaskan Peninsula. During June 1912, 8 cubic miles of fragmented molten rock erupted at the head of the Ukak River Valley in the most violent and voluminous eruption of the 20th Century. The valley has since become known as the "Valley of Ten Thousands Smokes" and the region dedicated as a National Park and Wilderness Area.

Teams consisting of 26 scientists in 1989 and 15 in 1990 studied and carefully measured such fundamental properties of the earth's crust as heat flow, gravity, magnetism, electrical resistivity, topography and structural geology to lay the groundwork for the scientific drilling phase to be undertaken in 1992. Extensive electrical and magnetic surveys were conducted in 1980 to supplement the previous year's data. Physical volcanological and hydrothermal geochemical investigations continued. Subject to meeting the requirements of the National Environmental Policy Act (NEPA), the granting of a drilling permit by the National Park Service, and the availability of funds for the purpose, the Katmai Scientific Drilling Project is ready to proceed with drilling in 1992.

This national program is 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 USGS in 1984. Under the terms of the Accord, DOE is responsible for the drilling and logistic activities associated with regions of abnormally high heat flow, such as Katmai, although each agency supports research on such projects as may be consistent with its range of interests and capabilities. Since it began scientific drilling in 1983, DOE has been leading the way in continental scientific 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 Geosciences Program also supports research in seismology both in furtherance of its objectives in high resolution underground imaging and in furtherance of its studies of volcanic hazards for energy facilities. In this connection, researchers at the University of Southern California and the University of California, Santa Barbara, report finding the first solid evidence for guided seismic waves propagating in the low-velocity layer of highly fractured rock associated with faults. In a paper published in Science, the researchers describe the detection and analysis of dispersive wave-trains associated with the Oroville and San Andreas fault zones, California. The low-frequency, low-velocity ringing effects detected within and close to the fault zone and other wave characteristics provide information on source mechanisms and fault-zone characteristics.

Finally, in the area of geological age-dating, an area of science important for energy resource studies, for global change, and for the isolation of hazardous wastes, earth scientists at the Los Alamos National Laboratory have developed a new analytical technique for measuring very low concentrations of thorium in geological samples that will have an important application in resolving the fine structure of global change over the past 300,000 years. The accuracy and precision of the uranium-thorium disequilibrium dating method is improved by three orders of magnitude because of highly efficient ionization of thorium by means of laser-induced resonance prior to mass spectrometric measurement. The new technique is especially applicable to very small samples or to samples with very low thorium content. It can be applied, for example, to the dating of ice cores, which usually contain trace amounts of uranium and thorium in dust from ancient volcanic eruptions, and to the dating of calcium carbonate in deep sea sediment cores and cave deposits. More accurate dates will be useful in understanding the reasons for the historical major global changes, as recorded in the ice, the cores, and the deposits.

More information on this subprogram can be obtained from James S. Coleman, Director, Division of Engineering and Geosciences, ER-15, Office of Basic Energy Sciences, Department of Energy, Washington, D.C. 20585, (301) 353-5822. There are two reports available which supply more detailed information: "Summaries of FY 1989 Engineering Research", DOE/ER-0436; and "Summaries of Physical Research in the Geosciences", DOE/ER-0430, December 1989.

Advanced Energy Projects

The Division of Advanced Energy Projects (AEP) administers the AEP subprogram, Heavy Ion Fusion Accelerator Research (HIFAR), and the Small Business Innovation Research (SBIR) program* of the DOE.

Advanced Energy Projects

The objective of the AEP subprogram is to explore the feasibility of novel energy-related concepts evolving from basic research. These concepts are typically at an early stage of scientific definition and, therefore, beyond the scope of ongoing applied R&D or technology programs. Exploratory concepts that do not readily fit into a program area but do appear to have broad potential applications also are supported. Concepts in the AEP subprogram usually involve a high degree of risk. However, each has the potential for high pay-off. Thus, AEP offers a unique mechanism within DOE for transitioning basic research results into technology applications.

Although projects are supported for a limited period of time, usually 3 years, the AEP subprogram is not limited to supporting projects in a particular technical area or from a particular sector of the technical community. Current projects cover a broad range of technology, e.g., novel light sources, with an emphasis on short wavelength (extreme ultraviolet and beyond), innovative methods for materials separation or for resource recovery and innovative methods for oilspill cleanup. AEP projects are pursued by investigators at universities, industrial laboratories (including small R&D companies), and national laboratories.

A standard for measuring success in the AEP subprogram is the transfer of a project to technology development programs following AEP support. A number of successful transfers have been made over the years. In 1988, a company called ParaMagnetic Logging, Inc. (PML), established the scientific feasibility of a new technique to be used in locating oil and gas deposits overlooked in existing reservoirs. The oil and gas industry measures the resistivity of geological formations to determine the presence of oil and gas in newly drilled holes. However, these measurements have been impossible to perform through the steel pipes (borehole casings) which surround wells in older oil fields. With funding from the AEP subprogram, PML developed a new technique to measure resistivity through such cased boreholes, allowing the detection of "missed oil" and "bypassed gas". As a consequence of this AEP support, PML was then able to attract funds from a consortium of sources for a

*See page 48 for a discussion of the Department of Energy's SBIR program.

project to construct and test an apparatus to demonstrate the technology in actual oil and gas fields.

In 1989, an AEP subprogram project called the Composite Optical/X-Ray Laser Microscope (COXRALM) received an R&D 100 Award. This concept obtains images of biological cells at higher resolution than could be achieved with the use of an optical microscope. This improved resolution is possible by operating at a wavelength much shorter than that used in optical microscopes. The light source used is a soft X-ray laser (SXL) producing short pulses of high intensity, well collimated radiation. The COXRALM/SXL could eventually provide researchers with a unique capability for imaging biological specimens.

Heavy Ion Fusion

The HIFAR program is not subject to the prevailing 3-year funding limit. Heavy ion fusion emerged during the early phase of inertial fusion research, which had been developing laser and particle beam "drivers" to direct energy onto pellets of tritium and deuterium under conditions needed to achieve a fusion reaction. Recent advances in accelerator technology and in understanding beam transport have increased the attractiveness of using heavy ion beams to produce electricity from inertial fusion. A major issue awaiting technical resolution is whether beams of heavy ions can be generated at the intensities required for fusion in a cost-effective manner.

HIFAR is a research effort in accelerator science and technology that was spun-off in 1983 from the now defense-oriented DOE inertial fusion program. The HIFAR objective is to establish a data base sufficient to support a future, informed decision on whether or not to move forward with this method for inertial fusion. The HIFAR strategy is to address as many driver features as possible through a sequence of scaled experiments of increasing size and complexity. The HIFAR effort is centered at the Lawrence Berkeley Laboratory. Supporting activities are underway at the Lawrence Livermore National Laboratory and the Stanford Linear Accelerator Center.

Additional information can be obtained from Walter M. Polansky, Acting Director, Division of Advanced Energy Projects, Office of Basic Energy Sciences, ER-16, Department of Energy, Washington, D.C. 20585, (301) 353-5995. A summary report of ongoing projects, "Advanced Energy Projects FY 1990 Research Summaries," DOE/ER-0465T, September 1990, is available.

Energy Biosciences

The principal objective of the Energy Biosciences subprogram is to provide basic information and conceptual understanding in the microbiological and botanical sciences. This knowledge is important to DOE's efforts in renewable resource production of fuels and chemicals, microbiological transformation of organic materials, 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.

Micro-organisms that grow in the absence of oxygen and are able to carry out fermentations with high efficiency are of special interest, as are thermophilic micro-organisms, those having optimal growth and conversion rates at high temperatures. An integral part of the subprogram is the development of genetic information that may ultimately be used to produce new or improved micro-organisms and plants with properties that can be used to facilitate the production of fuels or petroleum-conserving chemicals or be used for new biotechnologies capable of conserving energy. Recent successes in introducing "new" genes into sulfate-reducing bacteria, lignin-degrading fungi, and barley plants are examples of genetic manipulation developed with program funds.

In 1986 the Energy Biosciences subprogram became involved in a multiple Federal agency effort to encourage plant-related research in the U.S. This has led to the establishment of several research centers in the U.S. whose goals are to address specific plant research areas. The Energy Biosciences subprogram is funding a center at the University of Georgia concentrating on the structure of complex carbohydrates. Complex carbohydrates not only comprise the major structural component in plants, but also function in numerous aspects of plant growth and development. Energy Biosciences also funds a center at Arizona State University that is focused on employing site-directed mutagenesis for producing mutants with defined protein changes to study the early biochemical and biophysical events in photosynthetic capture and conversion of light energy.

Recent accomplishments under this subprogram include:

1. ***Light Regulation of Photosynthesis*** -- Chloroplasts in plants are the receptors for the light energy used in the photosynthetic process. The chloroplasts undergo subtle biochemical and structural changes depending upon the quality of light they receive. This adaptability permits the same species of plant to thrive in a number of habitats with varying light conditions. During 1989, it was shown that the biochemical and structural changes in response to different colors of light do not result from changes in the reading of the genetic information contained in the DNA, but rather cause the rapid degradation of messenger RNA, an intermediate in the conversion of genetic information into proteins. Learning the manner in which environmental factors effect changes in the chloroplast's structure and biochemistry may offer a way of understanding basic control mechanisms present in plants that could lead to increased efficiencies to perform photosynthesis.

2. ***Development of Gene Transfer Technology for Sulfate-Reducing Bacteria*** -- Sulfate reducing bacteria convert sulfate (SO_4^{-2}) into H_2S during respiration instead of converting oxygen to H_2O as normally occurs in larger organisms. These organisms play critical roles in the global sulfur cycle, metal corrosion, and in oil well souring, sewage treatment and other fermentation processes that take place in oxygen depleted environments. While there has been considerable progress in learning about specific steps in sulfate respiration in the sulfate-reducing bacteria, the integration of these steps and the integration with the rest of the biological processes occurring within the bacteria has not been studied. A virus has been discovered with the ability to transfer genes between various strains of sulfate-reducing bacteria. Bits of DNA from the host cell are mixed in with the viral DNA when the virus is formed. When the virus infects another bacterial cell, the DNA is released in the new host cell and is incorporated into the genetic material of the new cell. The discovery of this system constitutes a major

development in genetically characterizing these organisms. While a system that would permit the genetic transformation of these organisms (the introduction of totally foreign DNA into the bacterial chromosome) is still being sought, the development of the viral transfer system has made possible extensive genetic studies on these important organisms.

3. ***Novel Gene Found In Methane Producing Bacteria*** -- The analysis of the structure or sequence of a particular gene or chromosome region sometimes gives insights beyond those which were originally planned. Such an example was the discovery, in the course of studies of the gene sequences encoding enzymes involved in the formation of methane in methane-producing bacteria, of a gene sequence for which no function was known. By comparison of this gene to other gene sequences cataloged in the GenBank data base, it was discovered that the gene has the information for the synthesis of a polypeptide that could best be described as polyferridoxin. The polypeptide should have the capacity to readily accept and give up six electron pairs. The physiological role of this molecule is not known, but there are several intriguing possibilities. These include behaving as a biological capacitor, being the equivalent of a biological electric wire, or serving as a ferridoxin precursor molecule. Studies are now underway to determine the biological role of the 'polyferridoxin' molecule in methane-producing microbes.

4. ***Visible Markers for Genetically Transformed Plants*** -- The technology available to insert foreign genes into one-celled organisms or cells permits success rates of incorporation varying from one in one thousand to one in ten million. The minuscule size of individual cells means that millions may be treated at one time. The major limitation becomes one of finding the cell which has received the foreign DNA. There is a high probability that adjacent genes will be incorporated together, particularly if the genes are small. A small gene with a rather pronounced effect, called a marker gene, is critical for genetic engineering applications.

Scientists at the University of Georgia, in collaboration with Pioneer Hi-Bred Seed Company researchers, have demonstrated that the R gene, which controls the synthesis of the purple pigment, anthocyanin, can be used as a marker to select for the incorporation of DNA into corn cells. The research involved placing the R gene into a piece of DNA. The DNA was then coated onto microscopic pellets and literally shot into corn tissue. The pellets are so small that they are able to enter a single cell without damaging it. After several days, purple cells could be readily observed showing that the R gene was functioning. These cells could be seen to divide with the daughter cell being purple showing that the gene had been incorporated into the corn chromosome. This technology, when combined with the recent accomplishments in regenerating whole corn plants from single cells, will permit ready genetic engineering of corn plants for research and commercial applications.

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

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

Small Business Innovation Research Program

The Small Business Innovation Research (SBIR) program, which is mandated by the Small Business Innovation Development Act of 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 grant applications on advanced concepts relevant to important energy-related scientific or engineering problems and opportunities that could lead to significant public benefit if the research is successful.

As prescribed in the legislation, the 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 as amended, which specifies that agencies subject to this law, of which there are 11 at present including DOE, spend certain percentages of their extramural research or R&D funds on SBIR projects. The law specifies 1.25% for each fiscal year from 1986 through 1993. On this basis, the DOE budget for SBIR is approximately $39 million in FY 1990. The budget for DOE's Defense Programs is exempt from participation in SBIR.

The Department issues SBIR program solicitations annually, with research or R&D opportunities provided each year in about 30 topical areas. The slate of topics 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 nondefense 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 8 years of the program, 1983-1990, 9,009 Phase I proposals were received and 984 Phase I awards were made. Three hundred seventy-two Phase II awards were made through FY 1990. The award selections have been made on the basis of scientific and technical excellence of the proposals.

Additional information about this program is available from Samuel Barish, SBIR Program Manager, ER-16, Department of Energy, Washington, D.C. 20585 (301) 353-3054. Reports containing abstracts of the projects receiving support are available. The current reports are "Abstracts of Phase I Awards, 1989, DOE/ER-0417" and "Abstracts of Phase II Awards, 1989, DOE/ER-0418." The most recent program solicitation can be obtained by contacting the SBIR Program Manager.

Major BES Facilities

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. How neutrons are scattered by molecular structures provides a means of determining those structures and some of their properties. Neutron scattering techniques yield information on the fundamental properties and behavior of materials and chemical and biological substances which cannot be obtained by any other means. The HFBR is one of two high-flux research reactors supported by DOE, both of which are world-class research reactors for neutron research.

Current research using the HFBR includes studies of:

- The structure and dynamics of magnetic materials;
- The dynamics of materials as they change phase;
- Neutron irradiation effects on the physical properties of materials;
- The molecular structure and dynamics of 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; and
- The neutron spectroscopy of low-lying excited states in solids.

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

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

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

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

Recent accomplishments dependent on the availability of the HFBR include:

1. ***Magnetic Excitations in $YBa_2Cu_3O_6+x$*** -- Pioneering neutron scattering investigations of magnetism in the high T_c systems have been performed at Brookhaven National Laboratory beginning with La_2CuO_4, the first compound for which large single crystals became available, and continuing on Sr-doped crystals. In 1988, these studies were extended to the $YBa_2Cu_3O_6+x$ systems, for which the maximum superconducting transition temperature is 90 K at x = 1. Large single crystals with various oxygen contents have been grown by a group at the Institute for Molecular Science in Japan. Extensive neutron scattering measurements of magnetic excitations in these crystals have been performed in collaboration with researchers at the Massachusetts Institute of Technology. This work provided evidence for three-dimensional magnetic ordering in samples with low oxygen content, and evidence of a very strong magnetic coupling between copper atoms within the CuO_2 layers, the common structural element of these compounds. This research provided clear evidence that magnetism and superconductivity are closely associated in the layered copper oxide compounds.

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

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

<u>High Flux Isotope Reactor</u>
Oak Ridge National Laboratory
Oak Ridge, Tennessee

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

The HFIR cost about $15 million to build and attained its operating power of 100 MW in 1966 with a thermal flux in the target area of 2 to 5 x 10^{15} neutrons/cm^2-sec. It is a light water moderated reactor and has had an unsurpassed record of better than 90% of scheduled operation. HFIR has a unique, two-piece core, which is its fuel element; this core is about the size of a 30-gallon drum and is replaced after about 3 weeks of operation. In addition to isotope production activities and in-core irradiations, there are twelve research stations at the four experimental ports. The National Center for Small Angle Scattering Research associated with the HFIR was sponsored as a joint project of DOE and the National Science Foundation. This Center was moved to the NIST Reactor when HFIR was shutdown in 1986 for refurbishment due to radiation damage to the vessel. It has since been restarted and will operate at 85 MW.

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

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

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

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

Although the use of HFIR has changed direction over the years, with increased emphasis on neutron irradiation and beam research and radioisotope production for sales, 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.

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 H. A. Glovier, Research Reactor Division, ORNL, Oak Ridge, Tennessee 37831, (615) 574-8049.

National Synchrotron Light Source
Brookhaven National Laboratory
Upton, New York

The National Synchrotron Light Source (NSLS) is a unique user-oriented facility for advanced multidisciplinary research with synchrotron radiation -- highly intense radiation emitted by 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 the 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. The vacuum ultraviolet (VUV) ring is 44 meters in circumference. A common injector meets the high-current requirement (1.0 A) for both rings. The VUV ring has been used routinely for research since early 1984. It operates at 750 MeV. The X-ray ring operates at 2.5 GeV. Since there are 47 ports at the two rings with each port capable of supporting one to three experiments, the NSLS has the potential of running about 100 experiments simultaneously.

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

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

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

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

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

- Studies of the state and behavior of gases;
- Studies of the 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; and
- Magnetic structure of surface and near surface layers in materials.

Recent accomplishments requiring the unique capabilities of NSLS are:

1. ***New Techniques for Studying Magnetic Properties of Materials*** -- With the advance of intense, polarized X-ray beams from

synchrotron sources, the polarization, momentum, and energy dependence of X-ray scattering processes can now be used to investigate properties of condensed matter in ways that could not have been imagined with X-ray sources of the past decade. Brookhaven physicists, working in collaboration with scientists at AT&T Bell Laboratories, Cornell University, Rice University, and the Institut Laue-Langevin in France, pioneered new synchrotron techniques to study the magnetic properties of materials by X-ray scattering. Magnetic properties are of intense interest due to their importance to the computer and electronics industries in data recording materials and devices.

2. ***Nature of the Charge Carriers in Electron-Doped Copper Oxide Superconductors*** -- In 1988, a Japanese group discovered a new class of high temperature, copper-oxide superconductors having the chemical formula $Nd_{2-x}Ce_xCuO_4$. In contrast to the previously known systems, such as the 90 K superconductor $YBa_2Cu_3O_7$ in which the charge carriers are known to be "holes" (missing electrons) on oxygen atoms, the mobile charges in the new compounds appear to be electrons. To characterize the electronic structure near the copper atoms, $Nd_{2-x}Ce_xCuO_4$ was studied using X-ray absorption spectroscopy at the National Synchrotron Light Source. The data obtained indicated that the electrons added by replacing Nd with Ce tend to sit on the Cu atoms.

   Understanding the similarities and differences between the electron and hole-doped compounds is quite important for theorists who are trying to explain the mechanism of superconductivity in these unusual materials. While the layered copper oxide compounds have a symmetry such that one can create superconductors by doping with holes or electrons, the nature of the electronic states involved in each case appears to be quite different. Deciding which of the previously advanced theories of superconductivity are consistent with the new observations is presently a critical issue in this rapidly evolving subject.

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

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

Stanford Synchrotron Radiation Laboratory
Stanford University
Stanford, California

Basic Energy Sciences is responsible for operating the Stanford Synchrotron Radiation Laboratory (SSRL). The SSRL is one of several national facilities, and DOE's second one, for the utilization of synchrotron radiation for basic and applied research in chemistry, physics, biology, and materials science. The SSRL was expanded under the auspices of the National Science Foundation in partial response to a National Academy of Sciences report that pointed out the potential for research in the newly identified area of synchrotron radiation. The SSRL, which shares the Stanford Positron Electron Asymmetric Ring 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 produced by the 4-GeV storage ring SPEAR operated by the Stanford Linear Accelerator Center (SLAC). The SSRL is a user-oriented facility that welcomes inquiries and proposals for experiments from qualified scientists.

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 (Stanford Positron Electron Assymetric Ring) 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 1,000 eV;

- Dynamic studies of conformational changes in biological systems, using time dependent X-ray diffraction and fluorescence lifetime techniques;

- Development of anomalous diffraction as a broadly applicable tool of crystallography;

- Results in other areas such as topography, lithography, and microscopy; and

- Development of a method of non-invasive angiography for heart disease patients.

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

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

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

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

Current research activities at SSRL include:

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

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

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

More information can be obtained from K. M. Cantwell, SSRL, Bin 69 P. O. Box 4349, Stanford, California 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 second) of the proton accelerator. High-energy protons from a proton synchrotron impinging on a heavy metal target produce bursts of neutrons knocked out of the target; these are called spallation neutrons. The resulting pulsed beams of neutrons, exploited using time-of-flight techniques, have the following characteristics:

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

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

- Static and dynamic properties of liquids and amorphous solids;
- Defects, voids, and aggregates in materials;
- Structure and dynamics of polymers and biological material;
- Magnetic, crystallographic, and electronic changes;
- Phonon structure and magnetic excitations in solids;
- Surface phenomena and superconductivity; and
- Radiation damage at cryogenic temperatures.

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

The IPNS, which began operation in FY 1981, has a peak thermal flux of 3 x 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 x 10^{12} neutrons/cm^2-sec. The proton current is 8 microamps providing 500 MeV protons in 30 bursts per second of 2 x 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.

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

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

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

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

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

Combustion Research Facility
Sandia National Laboratory
Livermore, California

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

- Detection and measurement in flames of short-lived reactive intermediates in key combustion reactions;
- Energy transfer process and chemical kinetics of molecules of combustion interest;
- Laser velocimetry to study turbulence effects in an internal combustion engine; and
- In situ laser diagnostics of the interactions of materials surfaces with flames.

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

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

Participants in the visiting-scientist program work at the facility for 2 weeks or longer. Research by these scientists is usually carried out in collaboration with members of the permanent staff; however, visitors may also bring their own experimental apparatus and take advantage of the special diagnostic capabilities available at the CRF. Sandia National Laboratory normally covers costs associated with development including, currently, a chopper spectrometer and a low Q diffractometer.

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

Combustion Research Facility
Sandia National Laboratory
Livermore, California

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

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

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

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

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

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

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

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

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

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

New Facilities

Two new light sources are under construction: at LBL a light source in the ultraviolet wavelength regime (1-2 GeV, Advanced Light Source); and at ANL a light source in the X-ray wavelength regime (6-7 GeV, Advanced Photon Source).

Design is underway for a new high-flux neutron source at ORNL, the Advanced Neutron Source.

Other Facilities

High-Voltage Electron and Atomic Resolution Microscope Facilities

High-Voltage Electron Microscopes (HVEM's) are invaluable for energy-related research important to 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 HVEM's 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 higher accelerating voltages, and instrumentation was incorporated so that the microscope could operate with minimum aberration over its entire voltage range (400 to 1,000 KeV). At its maximum voltage (1 MeV), the ARM has a point-to-point resolution of l.7 A (although 1.5 A 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.

The Kratos EM-1500 HVEM is designed primarily for dynamic in situ studies, but it can also resolve structures at the 3 A 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 2.4 A. Specimens for this microscope are restricted to 2.3 mm in diameter to fit into the ultra-high 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 20 A -- 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 l.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 3.5 A. 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 $2.5x10^4$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 10 amperes for protons to 0.1 amperes 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 which 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.

Program and Budget Trends

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

The new knowledge generated becomes part of the body of information upon which the applied technologies rest.

While research to broaden the technology base needed for specific individual energy technology options is extremely important, so also is our need for basic research to build the science base 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 1986, the following Basic Energy Sciences Program and Budget Trends have emerged:

- Increased importance to U.S. science of BES' major user facilities as national assets available to industrial as well as academic researchers;
- Enhanced efforts to foster communication of scientific results to technologists, for increasing the awareness of BES-supported researchers of scientific issues facing technologists, and the importance of rapid technology transfer to the private sector;
- 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, with particular emphasis on modernization and assurance of environmental, health and safety for such facilities;
- Increased focus on inter- and multi-disciplinary research activities.

The budget for FY 1990 is approximately $564.2 million (Table I) of which $36.5 million is for capital equipment and $76.8 million is designated for construction. The budget request to Congress for FY 1991 is $648.6 million.

Table 1. Office of Basic Energy Sciences Budget

Operating Expenses (by Subprogram)	Estimate FY 1990	Request FY 1991
Materials Sciences	196.2	221.9
Chemical Sciences	138.5	150.5
Applied Mathematical Sciences	43.2	48.0
Engineering and Geosciences	32.8	32.5
Advanced Energy Projects	14.4	24.0
Energy Biosciences	20.4	20.2
Program Direction	5.4	6.5
Subtotal	450.9	503.6
Capital Equipment	36.5	37.0
Construction	76.8	108.0
Total	564.2	648.6

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

Table 2 presents a breakdown identifying the major performers who carry out the Basic Energy Sciences program. About 73% of the program is conducted at the national laboratories including Lawrence Berkeley Laboratory (LBL) and Ames Laboratory, 25% at universities throughout the country, and the remainder elsewhere, including nonprofit institutions and industry.

Table 2. Major Performers

Laboratory	**73%**
University	**25%**
Industrial/Other	**2%**

Ames Laboratory and Lawrence Berkeley Laboratory are co-located with universities (Lawrence Berkeley at the University of California, Berkeley, and Ames at Iowa State University) and receive 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 postdoctoral students.

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

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

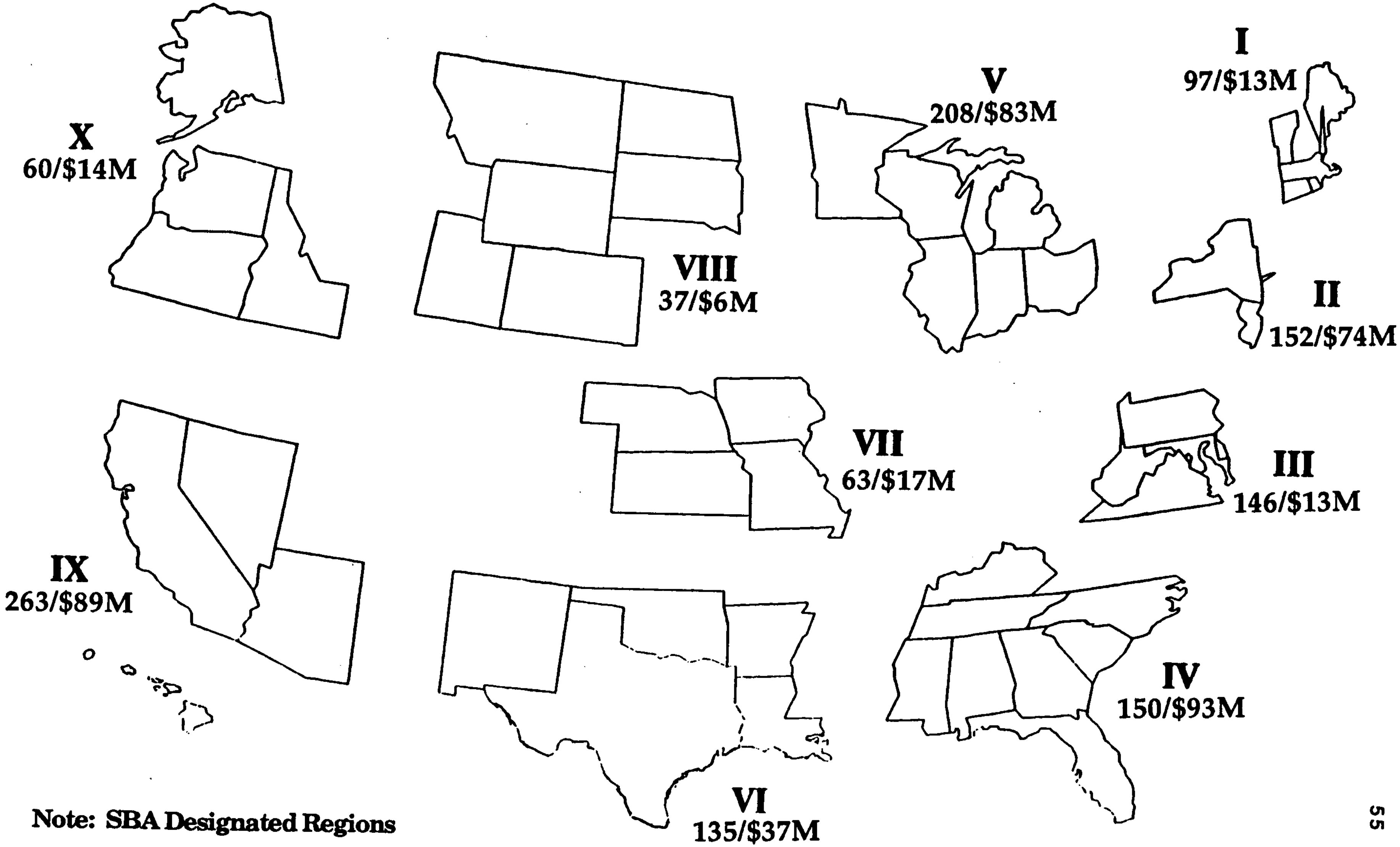
- *Surfaces* -- modification, interfaces, reactions at surfaces;
- *Solids* -- properties and structure, including grain boundaries, condensed matter theory, atomic transport, amorphous materials, structural ceramics;
- *Plants* -- genetics, response to stress, photochemistry;
- *Rock/fluid systems* -- underground imaging, rock/fluid interactions, isotope geochemistry;
- *Multiphase flow* -- transport properties of gas/liquid and other multiphase systems; and
- *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' 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.

The Basic Energy Sciences program is a major force in the Nation's overall strategy for research. During the past fiscal year, FY 1990 ending September 30, 1990, BES supported over 1,300 projects at universities, DOE laboratories, and other institutions. This research was reported in over 11,000 publications available through the open literature. Over 2,300 graduate students, 2,000 professors and post-doctoral scientists, and

1,800 full-time equivalent senior scientists at DOE laboratories were supported. The research was conducted in about 200 institutions throughout the United States. Figure 2 shows the number and operating dollars of BES projects distributed by regions of the country.

Figure 2.
Number and Dollars, Regional Distribution of BES Research Projects FY 1990



Note: SBA Designated Regions

Information Source Summary

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

Materials Sciences: Iran L. Thomas, Director, Division of Materials Sciences, ER-13, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-3427. Report available: Materials Sciences Programs Fiscal Year 1989 (DOE/ER-0447P) which summarizes current projects.

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

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

Engineering and Geosciences: James S. Coleman, Director, Division of Engineering and Geosciences, ER-15, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-5822. There are two reports available: Summaries of FY 1989 Engineering Research, DOE/ER-0436; and Summaries of Physical Research in the Geosciences, DOE/ER-0430, December 1989. Both provide detailed summaries of current projects.

Advanced Energy Projects: Walter Polansky, Acting Director, Advanced Energy Projects Division, ER-16, Office of Basic Energy Sciences, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-5995. Report available: Advanced Energy Projects FY 1990 Research Summaries, DOE/ER-0465T, September 1990.

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

Small Business Innovation Research: Samuel Barish, SBIR Program Manager, ER-16, U.S. Department of Energy, Washington, D.C. 20585, (301) 353-3054. Reports available: Abstracts of Phase I Awards, 1989, DOE/ER-0417, and Abstracts of Phase II Awards, 1989, DOE/ER-0418. The most recent program solicitation can be obtained by contacting the SBIR Program Manager.

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

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

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

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

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

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

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

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