U.S. DEPARTMENT OF ENERGY | Office of Science

Decades of Discovery

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1 INTRODUCTION

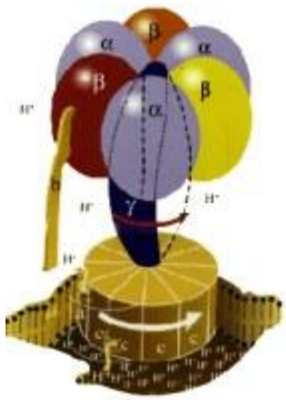
U.S. Department of Energy's
Decades of Discovery

For the past two-and-a-half decades, the Office of Science at the U.S. Department of Energy has been at the forefront of scientific discovery. We asked our staff and colleagues to help us identify 100 or so of the most important discoveries supported by the Office of Science.

The following list of discoveries is grouped by general discipline—the numerical order is random and not ranked by importance.

2 BASIC ENERGY SCIENCES

2.1 Adenosine Triphosphate: The Energy Currency of Life



Enzymatic mechanism of ATP synthesis

The energy cycle of all living organisms involves the molecule adenosine triphosphate (ATP), which captures the chemical energy released by the metabolism of nutrients and makes it available for cellular functions such as muscle contraction and transmission of nerve messages. A hard-working human adult can convert almost a ton of ATP daily. From the early 1960s through 1994, the Office of Science supported Paul D. Boyer's research at the University of California at Los Angeles on ATP synthase, the enzyme responsible for synthesizing ATP. His research examined the detailed chemical reactions involved in ATP synthesis and how the enzyme uses energy to create new ATP. Boyer theorized that this "molecular machine" with rotating parts functions in a surprising way for enzymes, a mechanism later supported by the work of John E. Walker of the United Kingdom. Among other things, Boyer discovered that energy input was not used primarily to form the ATP molecule, but rather to promote the release of an already formed and tightly bound ATP. Boyer and Walker shared half of the 1997 Nobel Prize in Chemistry for these achievements.

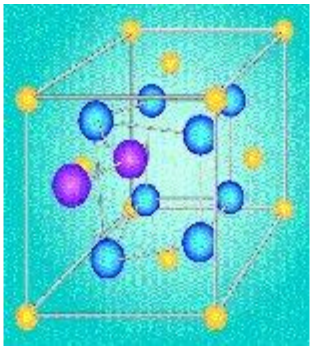
Scientific Impact: This work uncovered new concepts in enzymology and advanced understanding of how living cells function at the molecular level. Determination of how cells store and transfer energy has been among the most important advances in molecular and cell biology, enabling an entire generation of work at the cellular level in animal and plant research.

Social Impact: Research in cell biology has led to tremendous advances in medicine and physiology, such as clues to the genesis and treatment of cancer.

Reference: Boyer, P.D., "The ATP synthase—a splendid molecular machine," *Ann. Rev. Biochem.* 1997; 66:717-49.

SC-Funding Office: Basic Energy Sciences

2.2 Making Better Catalysts



Model for Ceria Oxide System. Ceria atoms are yellow, oxygen atoms are blue, and the active oxygen at the defects are purple.

Catalysts, which accelerate chemical reactions, are valuable in many industries, from fuels to pharmaceuticals. Long-term research by government and academic scientists supported by the Office of Science has led to new understanding of catalytic phenomena, in particular the relationship between chemical structure and reactivity. For example, early work established two classes of heterogenous catalysts (which function by adsorbing molecules), based on whether chemical reactivity is, or is not, sensitive to surface structure. These studies showed that catalytic reactions once thought to be structurally insensitive actually took place on a dynamic surface. Research on the reactivity of hydrogen with catalysts—an issue in the world's largest-scale industrial processes, such as sulfur removal from crude oil-disproved the widely held belief that hydrogen molecules must dissociate into two atoms before undergoing reactions, and challenged the accepted notion that surface-bound (as opposed to embedded) hydrogen was the only reactive form. Other discoveries concerned the chemical behavior of organometallic complexes (combinations of organic and metallic species) that are used, for example, in plastics manufacturing.

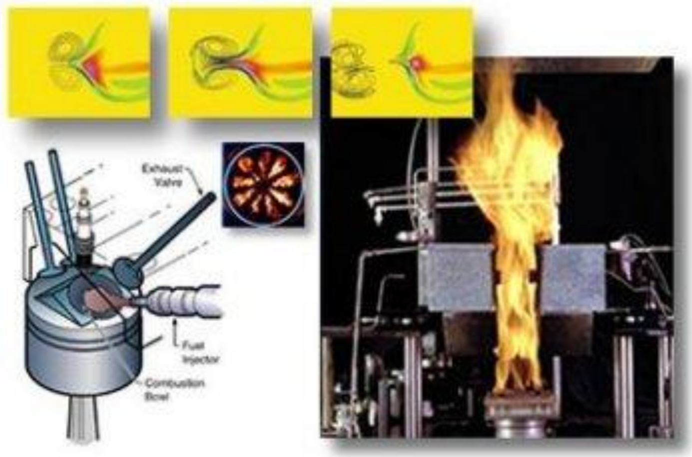
Scientific Impact: Research on structure-reactivity relationships has increased understanding of both natural and synthetic processes. The discovery of nonclassical binding of molecular hydrogen created a new field of study that may overcome some of chemistry's greatest challenges, such as conversion of natural gas to more usable liquid fuels (methanol or gasoline).

Social Impact: A modern society's standard of living can be measured by its accomplishments in catalysis, because every manufacturing process and energy-generating technique starts with catalysis. Catalysts first introduced by investigators supported by the Office of Science revolutionized a process used to make about 100 billion pounds of plastics per year worldwide; this work is leading to catalysts that produce superior plastics with new properties.

Reference: C.E. Tripa and J.T. Yates, Jr. Nature, 398 (1999) 591.

SC-Funding Office: Office of Basic Energy Sciences

2.3 Understanding Chemical Reactions



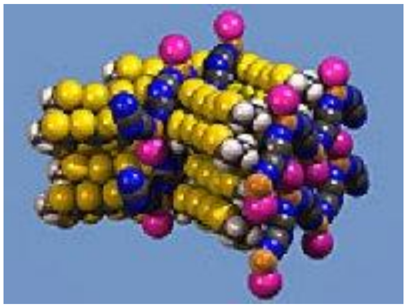
The molecular features that influence the rate of chemical reactions were poorly understood until the mid-1960s, when Dudley Herschbach and his postdoctoral student Yuan T. Lee began a series of experiments at Harvard University. With funding from the Office of Science and predecessor agencies, they explained in detail how chemical reactions take place, and solved the problem of how to observe the random directions and velocities of molecules in a gas or a liquid. They developed an apparatus in which crossed molecular beams were used to vary the velocities and approach angles of reacting molecules. With this tool, the scientists discovered and studied long-lived complexes of reactants formed before a reaction was completed, and described theoretically their formation and decay. They also examined the velocities of products, rotational energies, and internal vibration energies. In this way, they could map out all the details of a chemical reaction and explain the effects of temperature and pressure. Initially, these studies focused on reactions between alkali atoms and other molecules; Lee later adapted the crossed molecular beam method for general reactions. The 1986 Nobel Prize in Chemistry was awarded jointly to Herschbach, Lee, and a third scientist.

Scientific Impact: This work contributed significantly to the modern knowledge base for atmospheric and combustion chemistry. These scientists helped establish reaction dynamics as a discrete field of research, and their crossed molecular beam approach is among the most important contributions to this field.

Social Impact: These studies contributed to improvements in industrial production efficiency and assisted in the design of new products to be more useful, durable, and conserving of natural resources. This work also contributed to the development of predictive theories and models used to design and manufacture new products ranging from plastics to pharmaceuticals.

SC-Funding Office: Office of Basic Energy Sciences

2.4 New Types of Superconductors



Organic superconductor with the highest T_c k-$(ET)_2Cu[N(CN)_2]Cl$

Superconductors conduct electricity with little or no resistance. Organic superconductors contain carbon and are less dense than their ceramic or metallic counterparts; they also offer unusual potential for fine-tuning of electrical properties. Argonne National Laboratory long has carried out the major U.S. effort to synthesize and identify organic superconductors. Nearly 100 new superconductors of this type have been produced, with critical temperatures (at which a superconductor loses all electrical resistance) as high as -260 degrees C, or -434 degrees F. Recently, the first superconductor composed entirely of organic components (with no metal atoms) was synthesized, with a transition temperature in this range. Although this remains far lower than the highest known transition temperature for ceramics, scientists still expect that a high-temperature organic superconductor may be possible, such that liquid nitrogen (at -196 degrees C, or -321 degrees F) could be used as the coolant instead of the more costly liquid helium, thus making practical applications more feasible. The new compound has a two-dimensional, layered structure, which may provide significant insight into the nature of superconductivity.

Scientific Impact: These advances will help scientists develop a theory of how organic superconductors work and contribute to the design of new materials with higher transition temperatures. The all-organic material is ideal for studies of magnetic and charge transport properties because there is no possibility of contamination from metallic impurities.

Social Impact: Superconductivity already has important applications, such as medical diagnostic equipment, and many more uses are possible if transition temperatures are high enough. The availability of purely organic superconductors greatly expands the possibilities, especially for applications in which weight is a factor.

Reference: Ambient-Pressure Superconductivity at 2.7 K and Higher Temperatures in Derivatives of beta$(ET)_2IBr_2$: Synthesis, Structure, and Detection of Superconductivity. Williams, J. M.; Wang, H. H.; Beno, M. A.; Emge, T. J.; Sowa, L. M.; Copps, P. T.; Behroozi, F.; Hall, L. N.; Carlson, K. D.; Crabtree, G. W. *Inorg. Chem.* 1984, 23, 3839-3841.

A New Ambient-Pressure Organic Superconductor, kappa $(ET)_2Cu[N(CN)_2Br$, with the Highest Transition Temperature Yet Observed (Inductive Onset Tc=11.6 K, Resistive Onset=12.5 K) Kini, A. M.; Geiser, U.; Wang, H. H.; Carlson, K. D.; Williams, J. M.; Kwok, W. K.; Vandervoort, K. G.; Thompson, J. E.; Stupka, D. L.; Jung, D.; Whangbo, M.-H. *Inorg. Chem.* 1990, 29, 2555-2557.

From Semiconductor-Semiconductor Transition (42 K) to the Highest-T_c Organic Superconductor, kappa $(ET)_2Cu[N(CN)_2Cl$ (T_c=12.5 K) Williams, J. M.; Kini, A. M.; Wang, H. H.; Carlson, K. D.; Geiser, U.; Montgomery, L. K.; Pyrka, G. J.; Watkins, D. M.; Kommers, J. M.; Boryschuk, S. J.; Strieby Crouch, A. V.; Kwok, W. K.; Schirber, J. E.; Overmyer, D. L.; Jung, D.; Whangbo, M.-H. *Inorg. Chem.* 1990, 29, 3272-3274.

The First Organic Cation-radical Salt Superconductor (T_c=4 K) with an Organometallic Anion: Superconductivity, Synthesis and Structure of kappa $(ET)_2M(CF_3)4(C2H_3X_3)$. Schlueter, J. A.; Geiser, U.; Williams, J. M.; Wang, H. H.; Kwok, W. K.;Fendrich, J. A.; Carlson, K. D.; Achenbach, C. A.; Dudek, J. D.; Naumann, D.; Roy, T.; Schirber, J. E.; Bayless, W. R. *J. Chem. Soc., Chem. Commun.* 1994, 1599-1600.

Superconductivity at 5.2 K in an Electron Donor Radical Salt of Bis (ethylenedithio) tetrathiafulvalene (BEDT-TTF) with the Novel Polyfluorinated Organic Anion beta $(ET)_2SF_5CH_2CF_2SO_3)$ Geiser, U.; Schlueter, J. A.; Wang, H. H.; Kini, A. M.; Williams, J. M.; Sche, P. P.; Zakowicz, H. I.; VanZile, M. L.; Dudek, J. D.; Nixon, P. G.; Winter, R.W.; Gard, G. L.; Ren, J.; Whangbo, M.-H. *J. Am. Chem. Soc.* 1996, 118, 9996-9997.

SC-Funding Office: Office of Basic Energy Sciences

2.5 Development of Neutron Scattering Facilities

Powder Diffractometer High Flux Isotope Reactor (ORNL)

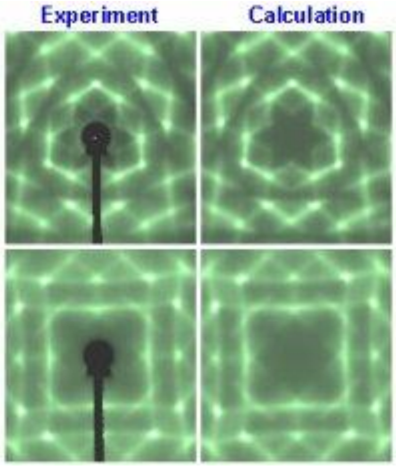
Neutron scattering provides key information on the positions, motions, and magnetic properties of solids. When neutrons flowing from a nuclear reactor bounce off atoms in a sample, the neutrons scatter in directions that depend on the atoms' relative positions in the sample structure. Changes in the neutrons' velocity provide information on the atoms' oscillations, or dynamics. Since the late 1940s, the Office of Science and predecessors have been major supporters of neuron science, including work by Clifford Shull and Bertram Brockhouse, who shared the 1994 Nobel Prize in Physics for their development of neutron scattering techniques for studies of condensed matter. Researchers at Oak Ridge, Brookhaven, and Argonne national laboratories developed neutron sources for spectroscopy, scattering, and imaging experiments and helped pioneer most of the associated instruments and techniques. The Office of Science currently supports three neutron sources—the High-Flux Isotope Reactor at Oak Ridge National Laboratory, Intense Pulsed Neutron Source at Argonne National Laboratory, and Manuel Lujan Jr. Neutron Scattering Facility at Los Alamos National Laboratory—used by hundreds of researchers annually. Under construction is a spallation neutron source at Oak Ridge that will be about an order of magnitude more powerful than any existing pulsed neutron source. Spallation produces neutrons with little heat; pulsed operation provides very high peak intensities.

Scientific Impact: Neutrons' unique properties, such as sensitivity to light elements, make them invaluable tools for polymer, biological, and pharmaceutical sciences. Studies made possible by neutron sources and the associated techniques contribute to the development of new materials, such as ceramic superconductors.

Social Impact: Neutron studies lead to new and improved products, such as powerful magnets for highly efficient electric motors. Also, because their high penetrating power allows nondestructive property measurements deep within a specimen, neutrons have been used to examine automotive gears and brake discs, and defects in aircraft wings, engines, and turbine blades.

SC-Funding Office: Office of Basic Energy Sciences

2.6 Development of Synchrotron Radiation Light Sources



Example shown is Si 111 (top) and Si 100 (bottom)

Synchrotrons produce a unique type of radiation—continuous across the spectrum and tunable to the desired wavelength—emitted by electrons accelerated in a magnetic field. For two decades, the Office of Science has been the major supporter of U.S. synchrotron light sources. It currently operates four, each with unique capabilities, used by a total of more than 6,000 researchers annually from academia, government, and industry. The four are the Advanced Light Source at Lawrence Berkeley National Laboratory, Advanced Photon Source at Argonne National Laboratory, National Synchrotron Light Source at Brookhaven National Laboratory, and Stanford Synchrotron Radiation Laboratory at Stanford Linear Accelerator Center. Scientists at these sites helped pioneer many synchrotron innovations that are widely used today, including a lattice of magnets that increased brightness (photon density) by two orders of magnitude; "insertion" devices (linear arrays of magnets called wigglers and undulators) that oscillate the path of the electron beam to generate X-ray and ultraviolet light that is high in flux (number of photons) and collimation (parallel alignment of photons); and powerful experimental techniques such as X-ray scattering and X-ray microscopy.

Scientific Impact: These innovations made new science possible and paved the way for significant extensions of light source performance that have had a broad and deep impact on the understanding of matter. Synchrotrons are used for cutting-edge research in materials science, physical and chemical science, geosciences, environmental science, bioscience, and medical and pharmaceutical science.

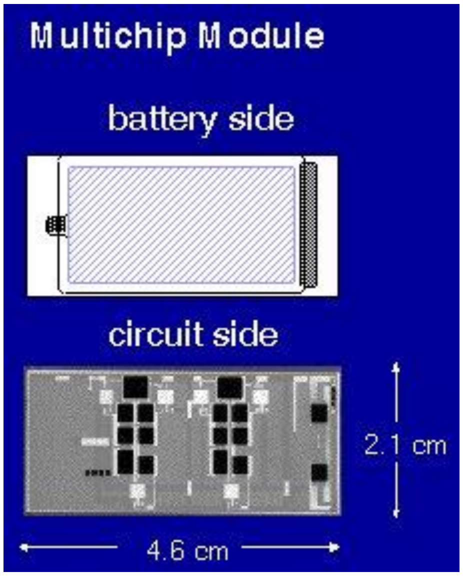
Social Impact: Synchrotron research affects society in areas such as information and energy technologies. For example, recent high-resolution imaging of thin films of copper may assist in the development of ultrahigh-density computer hard drives, and imaging of contaminants in solar cells and their removal by heat treatment may lead to more efficient and less costly solar energy.

Reference: P. A. Montano and H. Oyanagi, "In Situ Synchrotron Radiation research in Materials Science," *MRS Bulletin*, (24) 13-20 (January 1999).

W.Yun et al., "S-ray Imaging and Microspectroscopy of Plants and Fungi," *J. Synchrotron Rad.*, (5) 1390-1395 (1998).

SC-Funding Office: Office of Basic Energy Sciences

2.7 Development of Lithium Batteries



A thin-film Li-$LiCoO_2$ battery was fabricated onto the back side of the ceramic package of a multichip module. Contact with the circuit on the front side was made by depositing the cathode and anode current collectors over gold-plated through-holes. The battery was designed to supply 150 µAh between 4.2 and 3.8 V at a low current.

Lithium batteries, which offer both high energy-storage capacity and an environmentally benign alternative to the harmful lead used in conventional batteries, are based on research supported by the Office of Science and its predecessors. An early innovation was the development of organic solid electrolytes—essential because traditional water-based electrolytes could react with metals such as lithium to cause an explosion. (A battery consists of positive and negative electrodes separated by an electrolyte, through which ions, or charged atoms, flow.) Charles Tobias at Lawrence Berkeley National Laboratory led the search for nonaqueous solutions from which reactive metals, such as lithium (then used in fusion-type nuclear weapons), could be electrolytically deposited. He focused on cylic esters, including propylene carbonate, which today is used extensively in battery technology. The pioneering research included the purification of solvents to dissolve the electrolyte, solubility and conductivity measurements, and decomposition and electrodeposition tests. The Office of Science currently supports research on ion transport in solid polymer and glassy electrolyte systems, helping to lay the groundwork for the next generation of highly efficient and environmentally friendly batteries and fuel cells.

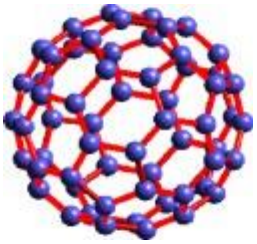
Scientific Impact: Tobias is widely regarded as the father of electrochemical engineering because he introduced scientific methods into a field formerly characterized by trial and error. His initial characterization of nonaqueous electrolytes, and demonstration that reactive metals could be electrodeposited from them, spawned a new field of battery research.

Social Impact: Lithium batteries are widely used in both consumer and defense applications, such as cellular telephones and notebook computers, but such batteries remain expensive. DOE applied research programs are developing new and less costly versions of rechargeable lithium batteries for use in electric and hybrid vehicles.

Reference: Dudney NJ, Bates JB, Lubben D, "Thin-Film Rechargeable Lithium Batteries," in *Role of Ceramics in Advanced Electrochemical Systems*. American Ceramic Society, 1996 p. 113.

SC-Funding Office: Office of Basic Energy Sciences

2.8 A New Class of Carbon Structures



A new allotrope of carbon that consists of 60 carbon atoms, shown above, in the shape of a soccer ball.

Several lines of research—in spectroscopy, astronomy, and metallic clusters—converged in 1985 to lead to the discovery of an unusual molecule. This cluster of 60 carbon atoms was especially stable because of its hollow, icosahedral structure in which the bonds between the atoms resembled the patterns on a soccer ball. The molecule was named Buckminsterfullerene after the geodesic domes designed by architect Buckminster Fuller. The identification of this form of carbon (also called buckyballs) sparked broad interest in the chemistry of an entire class of hollow carbon structures, referred to collectively as fullerenes. Formed when vaporized carbon condenses in an atmosphere of inert gas, fullerenes include a wide range of shapes and sizes, including nanotubes of interest in electronics and hydrogen storage. The initial discovery was recognized by the 1996 Nobel Prize in Chemistry, awarded to Richard E. Smalley and Robert F. Curl, both supported by the Office of Science, and Curl's colleague Sir Harold W. Kroto of Great Britain. More recently, scientists at Lawrence Berkeley National Laboratory reported a new synthetic method for producing, extracting, and purifying a cluster of 36 carbon atoms in quantities useful for research purposes; they also confirmed the high reactivity and other unusual electrical and chemical properties of this material.

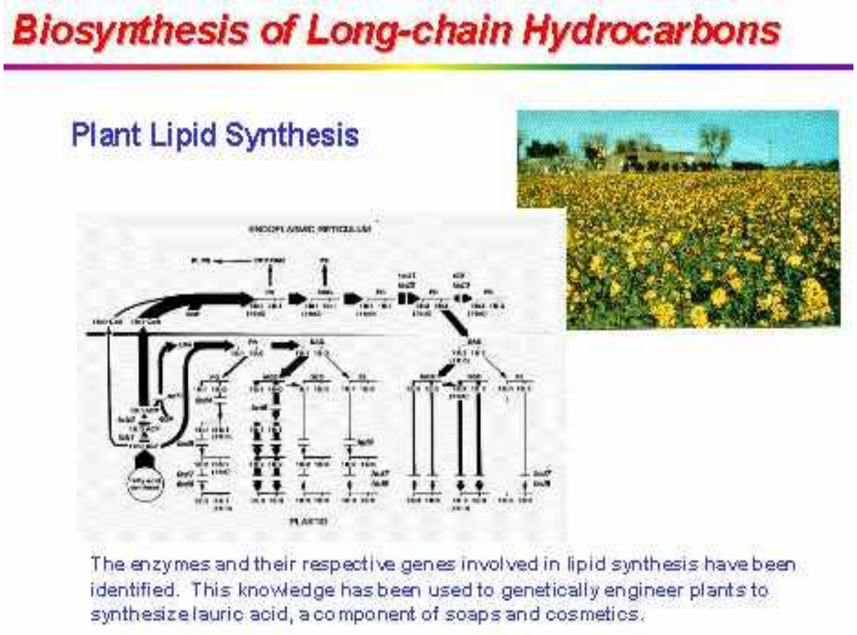
Scientific Impact: The discovery of fullerenes launched a new branch of chemistry, and related studies have contributed to growing interest in nanostructures in general and the principles of self-assembly. Fullerenes also have influenced the conception of diverse scientific problems such as the galactic carbon cycle and classical aromaticity, a keystone of theoretical chemistry.

Social Impact: Fullerenes are highly versatile (there are literally thousands of variations) and thus have many potential applications. For example, fullerene structures can be manipulated to produce superconducting salts, new three-dimensional polymers, new catalysts, and biologically active compounds.

Reference: "C60: Buckminsterfullerene," H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl, and R.E. Smalley, *Nature* 318, 162, November 14, 1985.

SC-Funding Office: Basic Energy Sciences

2.9 Engineering Organisms to Make Valuable Biomaterials



Plants and microbes are natural biochemical factories, producing important chemicals and materials. (Petroleum deposits are the altered remains of prehistoric plants and microbes.) The Office of Science long has supported basic studies on biochemistry and genetics that are providing insights into how plants and microbes can be modified to make more products with economic value. Christopher Somerville, while at DOE's Plant Research Laboratory at Michigan State University, demonstrated the capability to transfer an alignment of genes from bacteria to higher plants that confer the ability to synthesize biodegradable plastic components. He also studied the biosynthetic pathways for plant oils to learn what genetic changes would produce a different and more desirable type of oil. Research by Lonnie Ingram at the University of Florida focused on the regulation of genes that play critical roles in a bacterium's natural production of ethanol. He engineered DNA with genes for making two key enzymes; not only did this DNA alter the production pathway, but it also was incorporated into the genetic material of numerous other bacteria that did not normally form ethanol—and they started to make it.

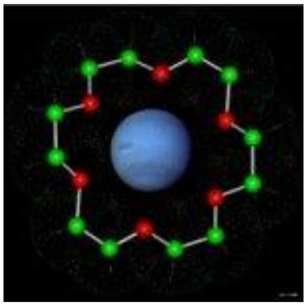
Scientific Impact: Somerville's work represents an early breakthrough in enhancing the use of plants as biosynthesizers of precursors for biodegradable plastics, which could replace products now derived from petroleum. Ingram's research suggests the potential for altering many bacteria, with many potential growth substrates, to produce ethanol.

Social Impact: Biosynthesis of compounds that can replace petroleum-derived products could reduce U.S. reliance on foreign oil. The University of Florida patented an ethanol-producing organism capable of growing on certain sugars, and an ethanol plant in Louisiana is demonstrating the commercial potential of a process based on this research.

Reference: Buchanan, B.B., W.Gruissem, and R.L. Jones, *Biochemistry & Molecular Biology of Plants*, American Society of Plant Physiologists (aspp@aspp.org), 2001.

SC-Funding Office: Office of Basic Energy Sciences

2.10 Heavy Element Chemistry



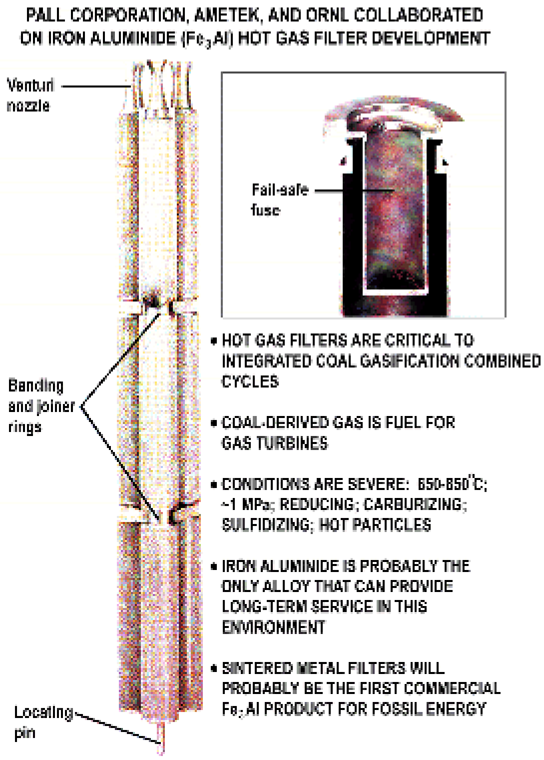
For more than 50 years, the Office of Science and predecessor agencies have supported the discovery and study of the actinide elements, in particular the transuranium elements-atoms that are heavier than uranium. Glenn Seaborg and Ed McMillan of the Lawrence Berkeley National Laboratory, 1951 Nobel Laureates in Chemistry for the discovery of plutonium and other actinide elements, began this quest. Today, the Heavy Element Chemistry program continues the pursuit for a fundamental understanding of actinide and fission product chemistry. The discovery and the exploration of the properties of the transactinides, elements heavier than the actinides, is also being undertaken and presents significant challenges since these elements decay to the lighter elements in minutes, seconds, or milliseconds. One of the leading researchers in this area is Darleane Hoffman of Lawrence Berkeley, whose work earned her the National Medal of Science in 1997 (the nation's highest scientific honor) and the Priestly Medal of the American Chemical Society in 2000. Hoffman contributed to the development of "atom at a time" chemistry which makes possible the study of heavy elements with half-lives of a minute or less. She was among the researchers to confirm the existence of the element seaborgium, named after Seaborg. Hoffman now is involved in an international collaboration to study the chemistry of the transactinides, work inspired by predictions of unexpected chemical properties caused by relativistic effects.

Scientific Impact: Research on the heavy elements yields the basic knowledge that can be used to develop new technologies and processes for the safe handling and disposition of these radioactive materials. For the transactinides, new "atom at a time" chemical techniques are being used to determine and compare their chemical properties to other known elements. The Office of Science heavy element chemistry program is the nation's sole effort addressing the fundamental science of the transuranium elements.

Social Impact: This research helps DOE carry out what is perhaps its most important and difficult responsibility—stewardship of the nation's nuclear science and technology. Studies of these elements and their fission products are needed to address the environmental consequences of the weapons programs and possible accidental release of nuclear materials.

SC-Funding Office: Office of Basic Energy Sciences

2.11 Improving Intermetallic Compounds



Intermetallic compounds (metallic materials composed of definite proportions of two or more elemental metals) resist oxidation and remain strong at high temperatures, making them useful for energy technologies. But until recently, these compounds were too brittle to be fabricated into conventional shapes using traditional methods. In 1981, Oak Ridge National Laboratory started a program to increase understanding of intermetallic compounds and develop scientific principles for improving their properties. Following a Japanese report suggesting that small amounts of boron made a nickel aluminide compound more ductile, Oak Ridge researchers led by Chain T. Liu determined the mechanism behind the change. They also showed that iron aluminides are intrinsically ductile at ambient temperatures and that brittleness is caused by moisture in the air. Quantum mechanical calculations demonstrated a mechanism that reduced the cohesive strength of atomic layers in these alloys by 70 percent, a discovery that led to new and improved alloy designs. Liu was awarded the 2001 *Acta Metallurgica* Gold Metal for his outstanding leadership and achievements in this research. The Office of Science then worked with DOE offices of Energy Efficiency and Fossil Energy to fund a research program on intermetallic compounds, an effort that has won three R&D 100 awards from *R&D Magazine* recognizing significant new technologies, and has resulted in more than 16 patents and 12 licenses.

Scientific Impact: Materials and processing research at Oak Ridge has increased scientific understanding of intermetallic compounds. This work overcame the brittleness problem and improved manufacturability, thus making it practical to use nickel and iron aluminides for high temperature engineering applications.

Social Impact: This research has helped to improve product quality and reduce costs. For instance, the use of nickel-aluminide dies for the hot forging process improves the quality of steel parts in automobiles, and iron-aluminide filters used to remove ash particles during coal gasification reduce costs and resist the corrosiveness of hydrogen sulfide in the gas stream.

Reference: Pope, D. P., C, T. Liu, S. H. Whang, and M. Yamaguchi, eds., *High Temperature Intermetallics*, Elsevier, New York (1997).

SC-Funding Office: Office of Basic Energy Sciences

2.12 Ion Beam Techniques Enhance Materials Science

Since the 1940s, Oak Ridge National Laboratory has played a leading role in the development of ion beam technology and its application in materials processing and characterization. A key advance was made in the early 1960s when, in one of the first applications of computers in materials science, researchers predicted that positive ions (charged atoms) moving through a crystal would follow channels between the rows of atoms, thereby penetrating well into the crystal structure. The "ion channeling" effect became the basis for valuable scientific and commercial processes used to force ions into materials as a means of tailoring or altering their properties. One such process is ion implantation, now developed into a fine art that relies on accelerators to drive selected ions into materials at precise distances. Many materials so modified are now in routine use. Today, Oak Ridge operates a facility where the broader scientific community carries out fundamental research on various ion beam techniques to selectively design the near-surface properties of materials.

Scientific Impact: Ion beam techniques are widely used for research on topics such as superconductivity, thin-film electrolytes, quasicrystals, and surface structure and chemistry. The science continues to evolve; new approaches to controlling the morphology and properties of ion-implanted materials and layers now are being developed based on defect physics.

Social Impact: Ion implantation is used extensively in the electronics industry to "dope" semiconductors with special properties, both chemically and spatially. The process is also used to improve the wear resistance of titanium alloys in artificial prostheses for hip and knee replacements. By eliminating the need to rework failed replacement joints, this technology spares individuals from additional surgeries and saves as much as $100 million per year.

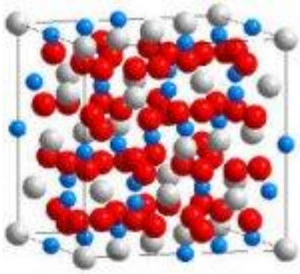
Reference: E. Chason, et al, "Ion beams in silicon processing and characterization," *Journal of Applied Physics*, vol. 81, no. 10, pp. 6513-6561 (1997) [Report of BES study panel]

A. Agarwal, H.-J. Gossmann, D. J. Eaglesham, S. B. Herner, A. T. Fiory, and T. E. Haynes, "Boron-enhanced diffusion of boron from ultra-low energy ion implantation," *Applied Physics Letters* vol. 74, pp. 2435-2437 (1999).

J. M. Williams and R. A. Buchanan, "Ion implantation of surgical Ti-6Al-4V alloy," *Materials Science and Engineering* vol. 69, pp. 237-246 (1985).

SC-Funding Office: Office of Basic Energy Sciences

2.13 Preventing Radioactive Contamination



Gadolinium zirconate is a highly radiation-resistant material that shows promise for use as a durable storage material for immobilizing plutonium and other actinides. The structure of gadolinium zirconate ($Gd_2Zr_2O_7$) above is color coded: Blue=Gadolinium (Gd), Gray=Zirconium (Zr), Red=Oxygen (O).

Worldwide, nuclear energy and weapons programs have created 1,350 metric tons of plutonium, an amount still growing by 70 metric tons annually. A major issue facing society is how to dispose safely of plutonium, which is radiotoxic and decays very slowly (it has a half-life of 24,500 years). One strategy is to immobilize it in chemically durable materials that absorb harmful neutrons and resist radiation damage. A 20-year collaboration between Rod Ewing at the University of Michigan and Bill Weber of Pacific Northwest National Laboratory has identified such materials. Using simulation techniques, they discovered that gadolinium zirconate materials resist radiation damage for millennia. These compounds absorb energy through the rearrangement of atoms within the crystal structure without becoming amorphous or structurally unstable—making them superior to the titanate materials being considered internationally for plutonium immobilization. (Plutonium-bearing titanates would degrade much faster.) The researchers also confirmed the mobility of the disturbed atoms and the ease of incorporating plutonium into the gadolinium-zirconate structure.

Scientific Impact: These studies demonstrated a systematic increase in radiation resistance as zirconium is substituted for titanium in gadolinium compounds. Discovery of these materials has stimulated research elsewhere, including Los Alamos National Laboratory, and led to identification of a phase that seems to be the best candidate for immobilizing plutonium.

Social Impact: This material offers a promising means of keeping future generations safe from the dual threats of radioactive contamination caused by plutonium decay, and the nuclear proliferation that might result from further use of the plutonium in weapons. Thus, this work may help resolve major dilemmas of the nuclear age.

Reference: S. X. Wang, B. D. Begg, L. M. Wang, R. C. Ewing, W. J. Weber, and K. V. Govidan Kutty, "Radiation Stability of Gadolinium Zirconate: A Waste Form for Plutonium Disposition," *J. Materials Research* 14 [12] (1999) 4470-4473.

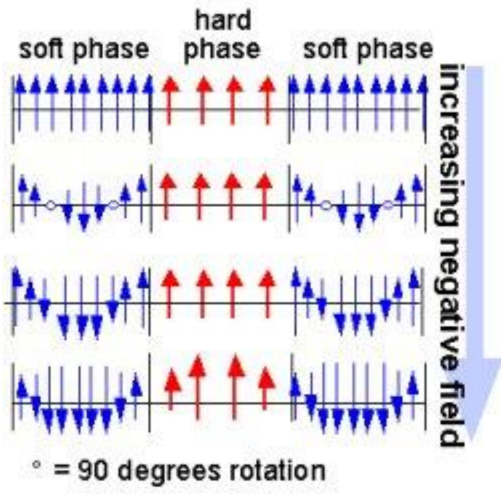
W. J. Weber et al., "Radiation Effects in Crystalline Ceramics for the Immobilization of High-Level Nuclear Waste and Plutonium," *J. Materials Research*, 13 [6] (1998) 1434-1484.

W. J. Weber and R. C. Ewing, "Plutonium Immobilization and Radiation Effects," Science 289 (2000) 2051-2052.

B. D. Begg, N. J. Hess, D. E. McCready, S. Thevuthasan, and W. J. Weber, "Heavy-Ion Irradiation Effects in $Gd_2(Zr_xTi_{1-x})_2O_7$ Pyrochlores," *J. Nuclear Materials* 289 [1-2] (2001) 188-193.

SC-Funding Office: Office of Basic Energy Sciences

2.14 Explaining and Applying Magnetism



Principle of Operation: Hard phase stiffens response of soft high-magnetization phase in magnetic nanocomposite structures.

Metallic magnetism is a time-honored field of study that in recent years has undergone a renaissance, thanks in part to Office of Science support. Research at Argonne National Laboratory on thin-film metallic multilayers is widely recognized as providing the basis for the discovery by others of giant magnetoresistance (GMR), an effect used widely today in recording heads in magnetic data storage devices. Related research has resulted in new GMR materials and structures, as well as contributions to the development and understanding of colossal magnetoresistance, a more powerful effect that may be used in future recording devices. Research at Brookhaven National Laboratory and Idaho National Engineering and Environmental Laboratory on hard magnets (permanently magnetized materials) explained the link between microstructure and properties in magnets made of rare earth materials; magnetic properties were improved dramatically through the design of microstructures on the nanoscale. Other work focuses on understanding and exploiting mixtures of hard and soft magnets with high magnetic strength. (The magnetization in soft magnets can be changed with applied magnetic fields.)

Scientific Impact: These studies have advanced the science of magnetic materials and paved the way for manufacture of magnet structures with greater mechanical strength and stability. Researchers benefit from these materials through their use in permanent magnet devices at Office of Science-supported synchrotrons and most other light sources around the world.

Social Impact: Magnetic materials are used in many industrial and consumer devices such as motors, generators, and computers. Improvements in magnet properties and processing characteristics will enhance energy efficiency; for example, the use of rare earth magnets in more efficient electric motors could save the nation several billion dollars annually.

Reference: L. H. Lewis, A. R. Moodenbaugh, D. O. Welch and V. Panchanathan, "Stress, Strain and Technical Magnetic Properties in "Exchange-Spring" Nd2Fe14B + a-Fe Nanocomposite Magnets", *J. Phys. D.: Appl. Phys.* 34 (2001) 744-751.

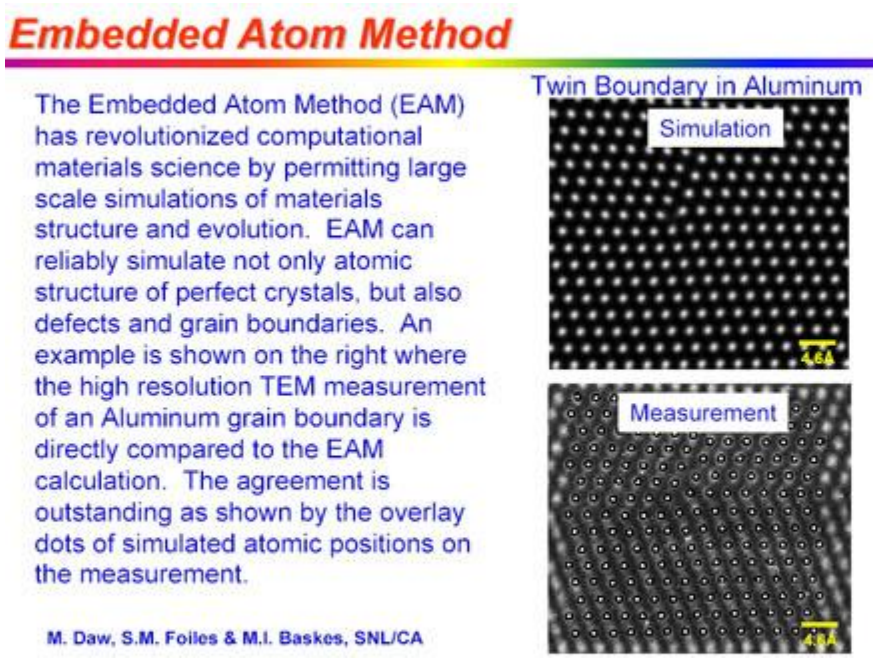
D. J. Branagan, M. J. Kramer, Yali Tang, R. W. McCallum, D. C. Crew and L. H. Lewis, "Engineering Magnetic Nanocomposite Microstructures", *J. Materials Science*, 35(14): 3459-3466, July 2000.

E. E. Fullerton, C. H. Sowers, J. E. Pearson, X. Z. Wu, D. Lederman, and S. D. Bader, "A General Approach to the Epitaxial Growth of Rare-Earth-Transition-Metal Films," *Appl. Phys. Lett.* 69, 2438 (1996).

E. E. Fullerton, M. J. Conover, J. E. Mattson, C. H. Sowers, and S. D. Bader, "Oscillatory interlayer coupling and giant magnetoresistance in epitaxial Fe/Cr(211) and (100) superlattices", *Phys. Rev. B* 48, 15755 (1993).

SC-Funding Office: Office of Basic Energy Sciences

2.15 Modeling Metals



For many years, scientists did not fully understand how and why metals and alloys sometimes cracked. The mystery was finally solved in the early 1980s, when Murray Daw and Mike Baskes at Sandia National Laboratories developed a way to accurately describe the embrittlement of steel by hydrogen or other corrosive impurities, a problem of interest in defense applications. Using concepts from density functional theory, they constructed the embedded atom method (EAM) from a "first principles" quantum mechanical framework for describing metal bonding. The EAM simplified the quantum behavior so that high-speed calculations could easily be made on very large systems containing hundreds of thousands of atoms. Whereas most fracture studies previously had been conducted on scales of inches or even feet, the EAM revealed much finer detail by focusing instead on atomic-scale processes, such as slight movements of electrons that weaken metal bonds. The EAM accurately describes important quantities such as cohesion and deformation of metals, making possible computer simulations that are useful in designing and predicting the behavior of complex materials and engineering components.

Scientific Impact: The EAM revolutionized computational materials science by enabling large-scale simulations of the atomic structure and evolution of metals; the method successfully simulates complex processes such as metal deformation, embrittlement, and fracture. The method is currently used by more than 100 groups worldwide and has resulted in more than 1,000 published works with more than 2,700 citations to the original paper.

Social Impact: The EAM is used in industry to design alloys for use in metallic parts and products.

Reference: "Parallel Molecular Dynamics With the Embedded Atom Method", S. J. Plimpton and B. A. Hendrickson, in Materials Theory and Modelling, edited by J. Broughton, P. Bristowe, and J. Newsam, *MRS Proceedings 291*, Pittsburgh, PA, 1993, p 37.

SC-Funding Office: Office of Basic Energy Sciences

2.16 Organic-Based Magnets: A New Frontier

Photograph of a coating of the V[TCNE]x magnet on a Teflon tape being attracted to a Co5Sm magnet at room temperature in the air.

Once considered to be a scientific impossibility, organic magnets (containing little or no metallic material) were discovered by chemist Joel Miller then at Du Pont, and physicist Arthur Epstein of The Ohio State University and both supported by the Office of Science. In 1986, they discovered the first organic material to become magnetically ordered (at very low temperature, -268 degrees C / -441 degrees F), demonstrating for the first time that a magnet could be made using organic chemistry and without the usual high temperature, energy intensive processing. (Magnetic ordering refers to the orientation of each atoms' electron spins, which behave like tiny magnets; when many adjacent electron spins align in the same direction, the material can be a strong magnet.) Miller and Epstein's compound is composed of molecular units. These are the first soluble as well as nonmetallurgically prepared magnets, and are more magnetic then iron metal. (Due to the high density of iron, organic magnets can never be as magnetic as iron on a volume basis.) Their research led to the 1991 discovery of the first organic/polymeric material to exhibit magnetism above room temperature, opening the door to many potential applications. More recently, the two researchers made thin magnetic films using a unique low-temperature process as well as another material that becomes magnetically ordered far above room temperature (~100 degrees C, or 212 degrees F). These accomplishments have been profiled on the covers of 15 journals and recognized by the *American Chemical Society's 2000 National Award for Chemistry of Materials*.

Scientific Impact: This work created a new class of materials and a thriving field of research that could lead to many new technologies. Since the original discovery, several new classes of polymeric organic magnets have been identified, and research consortiums have formed in both Europe and Japan.

Social Impact: Organic magnets are lighter, more flexible, and less energy intensive to make than conventional metal and ceramic magnets. Applications now being pursued include magnetic shielding, magneto-optical switching, and "smart" materials. The magnetic properties of these materials change when exposed to light, making them candidates for high-density optical data storage systems.

Reference: Ferromagnetic Properties of One-Dimensional Decamethylferrocenium Tetracyanoethylenide (1:1): [Fe(C5Me5)2] + [TCNE]. J.S. Miller, J.C. Calabrese, A J. Epstein, R.W. Bigelow, J. H. Zhang, W.M. Reiff, *J. Chem. Soc. Chem. Commun.* 1026-1028 (1986).

Organic and Organometallic Magnetic Materials - Designer Magnets, J. S. Miller, A. J. Epstein, *Angew. Chem. internat*. *edit*. 33, 385-415 (1994).

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A Room Temperature Molecular/Organic-Based Magnet, J.M. Manriquez, G.T. Yee, R.S. McLean, A. J. Epstein, J. S. Miller, *Science*, 252, 1415-1417 (1991).

Tetracyanoethylene-based Organic Magnets, J.S. Miller, A.J. Epstein, *J. Chem. Soc., Chem. Commun.* 1319-1325 (1998).

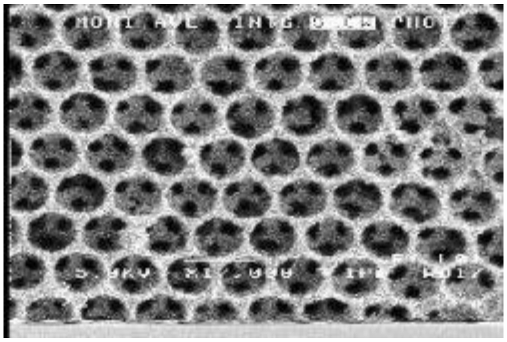
Thin Film V[TCNE]x Magnets, K. I. Pokhodnya, A. J. Epstein, J. S. Miller. *Adv. Mater.* 12, 410-413 (2000).

Enhancement of the Magnetic Ordering Temperature (and Air Stability) of a Mixed Valent Vanadium Hexacyanochromate(III) Magnet to 99 C (372 K), O. Hatlevik, W. E. Buschmann, J. Zhang, J. L. Manson, J. S. Miller, *Adv. Mater.* 11, 914-918 (1999).

Organometallic- and Organic-based Magnets: New Chemistry and New Materials for the New Millennium, J. S. Miller, *Inorg. Chem.* 39, 4392-4408 (2000).

SC-Funding Office: Office of Basic Energy Sciences

2.17 Manipulating Light in Photonic Crystals



A photonic band gap crystal produced by a colloidal crystallization technique using sized, template spheres.

Not long ago, theory and experiments failed to agree on the question of how light propagates in crystals. But in 1990, researchers at Ames Laboratory proved the theorists correct by demonstrating the existence of structures with a "photonic bandgap" (PBG), a range of frequencies within which a specific wavelength of light is blocked. Scientists then knew they could custom-design crystals to trap and manipulate light, sending it down assigned routes and even around loops and bends. Among their novel optical properties, PBG crystals can manipulate light without absorption; the energy not emitted in one frequency region is redirected into other frequencies, a useful feature in energy-efficient devices. Early photonic crystals had a bandgap in the microwave region of the electromagnetic spectrum. Using a layered lattice design and microfabrication capabilities at Sandia National Laboratories, scientists moved the bandgap to shorter wavelengths, in the infrared, for applications such as optical communications. Ames also produced computer programs that allow for the rapid design, analysis, and optimization of PBG structures.

Scientific Impact: The Ames' work spawned a growing global research community and knowledge base focusing on PBG crystals and related atomic properties and behavior. The high accuracy of Ames? theoretical calculations assists in the interpretation and design of PBG experiments and devices, and the layered lattice approach has been used to make the smallest PBG crystal ever fabricated.

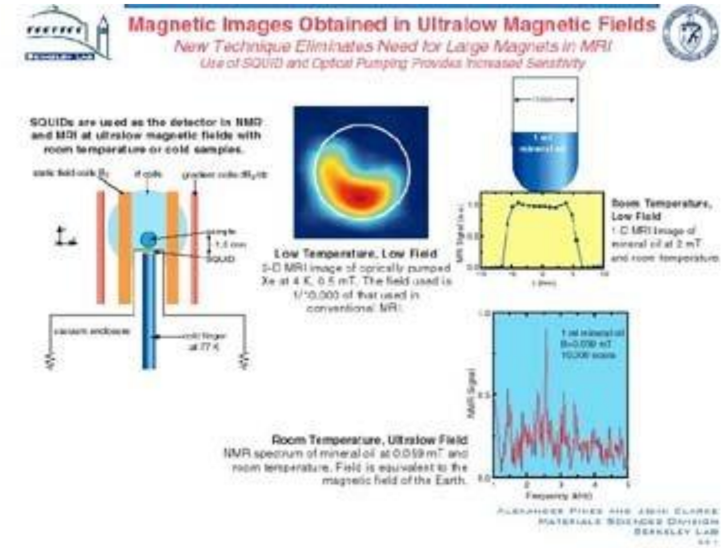
Social Impact: PBG crystals could revolutionize the control of light propagation, emission, and absorption in optical devices; thus, they have many potential uses in compact and efficient sensors, antennas, lasers, electronics, lighting, solar cells, and telecommunications equipment (e.g., optical switches, waveguides). The microfabrication method developed at Sandia is economical and lends itself to mass production.

Reference: "Photonic Crystals," M.M. Sigalas, R. Biswas, G. Tuttle, C.M. Soukoulis, and K.M. Ho, *Wiley Encyclopedia of Electrical and Electronic Engineering*, Volume 16, 345 (John Wiley, 1999).

"Existence of a photonic gap in periodic dielectric structures," K. M. Ho, C. T. Chan, and C. M. Soukoulis, *Phys. Rev. Lett.* 65, 3152 (1990).

SC-Funding Office: Office of Basic Energy Sciences

2.18 Extending the Power of Nuclear Magnetic Resonance Techniques



A larger .pdf version of this figure is available at the URL listed below.

Scientists at Lawrence Berkeley National Laboratory, led by Alex Pines, are world leaders in magnetic identification and imaging concepts and techniques used worldwide in science and industry. Both nuclear magnetic resonance (NMR) spectroscopy and magnetic resonance imaging (MRI) are based on the tiny magnetic moments produced by the "spin" of atomic nuclei; NMR provides spectra for use in identifying molecules, whereas MRI produces recognizable images. The Pines group's research has extended the applicability of NMR to a wide range of problems and materials, including biological systems. They also applied their new methods to study novel materials such as nanocrystals, liquid crystals, and zeolites. Recently, they helped develop a technique in which hyperpolarized gas molecules transfer added momentum to other atomic nuclei, increasing the sensitivity of NMR of molecules in solution and MRIs of materials and organisms, a major step toward extending the power of these techniques in chemistry and biology. The group also developed methods that allow for the use of very low magnetic fields in MRI and may eliminate the need for large, costly magnets in these instruments.

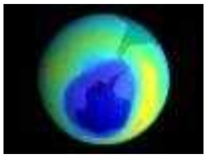
Scientific Impact: These novel concepts and techniques have revolutionized the study of structure, dynamics, and function in solid materials and other systems that previously were inaccessible to NMR investigations. Low-field MRI is ideal for studying highly porous, magnetic materials and fossils and rocks.

Social Impact: These techniques and instruments have been licensed and incorporated into commercial NMR technology used worldwide. A company has licensed the low-field MRI technology to develop medical applications. In addition, Pines has trained about 200 scientists, of whom many now hold leading positions in academia and industry.

Reference: Y.Q. Song, B.M. Goodson, and A. Pines, "NMR and MRI Using Laser-Polarized Xenon," *Spectroscopy*, (14) 26-33 (July 1999).

SC-Funding Office: Office of Basic Energy Sciences

2.19 Saving the Earth's Ozone Layer



The stratospheric layer of ozone 15 to 50 kilometers above the Earth absorbs ultraviolet radiation, preventing it from reaching the planet's surface. For many years, scientists assumed that this protective ozone would not be affected by release into the atmosphere of chlorofluorocarbons (CFCs), chemically inert and nontoxic gases once common in aerosol sprays and refrigerants. But in fact, CFCs do threaten the ozone layer, as explained in 1974 by F. Sherwood Rowland of the University of California, Irvine, and Mario Molina of the Massachusetts Institute of Technology. Rowland was supported by predecessors to the Office of Science for his research in hot-atom chemistry. Initially interested in species formed as a result of nuclear reactions, he extended his work to study the photochemical formation of chlorine atoms. Roland and Molina theorized that CFC molecules could be split apart by solar radiation to produce chlorine atoms, which could catalyze the destruction of ozone. They were right, as underlined later by discovery of the "ozone hole" over the Antarctic. Rowland and Molina, together with Paul Crutzen of the Max-Planck-Institute for Chemistry in Germany, shared the 1995 Nobel Prize in Chemistry for their work on the formation and decomposition of ozone.

Scientific Impact: Discovery of the effect of CFCs on the ozone layer was a seminal contribution to atmospheric chemistry.

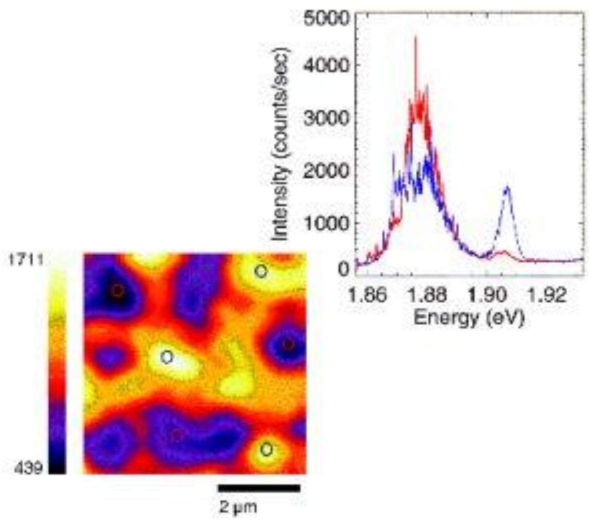
Social Impact: Rowland and Molina's work initially led to restrictions on CFC releases; after discovery of the ozone hole, an international agreement was signed to limit the manufacture and use of these compounds. Thus, this research has helped mitigate a global environmental problem with potentially catastrophic consequences. It will take at least 100 years for the ozone layer to recover fully.

Reference: Molina, M. j., and F. S. Rowland, Stratospheric Sink for Chlorofluoromethanes: Chlorine Catalysed Destruction of Ozone, Nature, 249, 810-814 (1974).

SC-Funding Office: Office of Basic Energy Sciences

2.20 Making Solar Energy More Affordable

Solar Panels



TEM Structure Analysis

The cost of solar electricity has been reduced 100-fold over the past two decades, but further reductions are needed before solar power is widely used. Scientists at the National Renewable Energy Laboratory took major steps toward this goal by designing photovoltaic cells (which convert sunlight to electricity) with 30 percent efficiency, much higher than the 10-20 percent levels achieved previously. The new cells consist of thin layers of semiconductors applied to a low-cost backing, such as glass or plastic. The researchers received Office of Science support to develop a basic understanding of the opto-electronic properties of various semiconductors. Calculations of electronic structure provided the knowledge needed to precisely engineer layered semiconductors. Then, a tandem device was designed with two solar cells made of materials that respond to different parts of the solar spectrum; the top cell (made of gallium indium phosphide) absorbs the high-energy component of sunlight and passes the rest to the bottom cell (made of gallium arsenide) for absorption. Researchers are working on the addition of a third cell to push efficiency to more than 40 percent, to open up new opportunities for terrestrial and space applications.

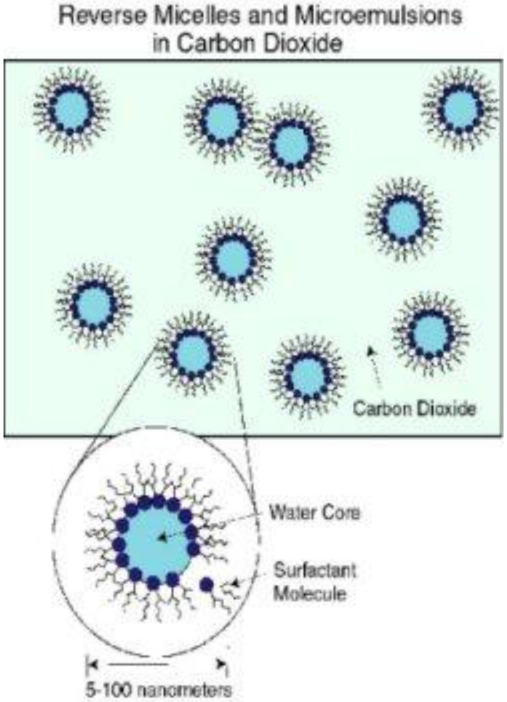
Scientific Impact: These advances have added to the scientific and engineering knowledge base needed to make solar power more practical and useful. For instance, the material used in the top layer of the new device is much more resistant to radiation damage than conventional silicon and thus will have a longer useful life.

Social Impact: The technology was transferred to a major supplier of photovoltaic cells for space power, and four satellites using it are in orbit, flashing back telephone and television signals. The new solar cells provide as much as 50 percent more power than previous cells, so the satellites can carry more communications links, experiments, or other projects and operate more economically.

Reference: Cotal, H. L.; Lillington, D. R.; Ermer, J. H.; King, R. R.; Karam, N. H.; Kurtz, S. R.; Friedman, D. J.; Olson, J. M.; Ward, S.; Duda, A.; Emery, K. A.; Moriarty, T. (2000). "Highly Efficient 32.3% Monolithic GaInP/GaAs/Ge Triple Junction Concentrator Solar Cells." *Program and Proceedings: NCPV Program Review Meeting* 2000, 16-19 April 2000, Denver Colorado. BK-520-28064. Golden, CO: National Renewable Energy Laboratory; pp. 111-112; NICH Report No. CP-520-29664.

SC-Funding Office: Office of Basic Energy Sciences

2.21 Enhancing Separations and Analysis



For many decades, the Office of Science and predecessor agencies have supported studies of the scientific principles underlying chemical separations and analysis. The most notable achievement was the development of the host-guest complexation concept by Donald J. Cram of the University of California, Los Angeles. This concept, which explains how molecules recognize and react with each other, changed how scientists think about separation and sequestration of elements. Cram also synthesized organic molecules that imitated the primary functions of enzymes, helping to fulfill a long-standing dream of chemists. For his pioneering work, Cram shared the 1987 Nobel Prize in Chemistry with two other scientists. Other researchers with Office of Science support developed inductively coupled plasma to produce sample materials for chemical analysis; wrote a powerful software program, SIMION, to help design particle beams and traps for fundamental studies; performed important basic research on supercritical fluids (liquefied gases used in solvent extraction); and developed laser-based detection schemes that enhanced the sensitivity of important analytical methods.

Scientific Impact: Cram helped to lay the foundation for one of the most active fields of chemical research, known as host-guest or supramolecular chemistry, which is directly applicable to separations. The work on inductively coupled plasma ushered in the era of ultra-trace multi-element analysis, enabling the rapid and accurate determination of up to 70 elements in metals, alloys, and organic compounds (such as oil, serum, blood, and soils). SIMION is used at every national laboratory.

Social Impact: Inductively coupled plasma is used in environmental testing and the production of ultrapure materials for the semiconductor and nuclear industries. The research on supercritical fluids contributed to the recent introduction of "green chemistry" for commercial dry cleaning and polymer manufacturing. SIMION is used by instrument suppliers that design mass spectrometers.

Reference: *DOE-BES Chemical Sciences, Highlights of Progress in Separations Sciences*, 1980-1999, Edited by Charles H. Byers, IsoPro International Inc., 2140 Santa Cruz Ave, #C304, Menlo Park, CA 94025 (http://www.sc.doe.gov/production/bes/chm/S&Ahistory/sephist.html)

SC-Funding Office: Office of Basic Energy Sciences

2.22 Sequencing the First Plant Genome

Arabidopsis thaliana

Arabidopsis thaliana, a small plant in the mustard family, has become the model for molecular genetic research on plants because of its small size, rapid growth cycle (6 weeks), large production of seed, and small genome (the smallest known of any flowering plant). In 1990, when *Arabidopsis* was being tested as a laboratory model for plant genetics, the DOE Plant Research Laboratory at Michigan State University initiated a project to analyze expressed sequence tags (ESTs), mirror images of fragments of genes and the proteins they make. Because they can be used to scan for and tag active genes, ESTs rapidly became important tools for identifying and isolating plant genes. Subsequently, other federal agencies provided support, resulting in a multinational computer database linked to U.S. and European stock centers, which distribute seeds and DNA of *Arabidopsis* to researchers worldwide. The research that grew out of this work laid the groundwork for the *Arabidopsis* Genome Initiative, which began 1996 as a multinational effort to sequence this plant's genome. The entire sequence (130 million pairs of chemical units) was officially completed recently and is largely available on the World Wide Web. As a direct model for 250,000 closely related species, *Arabidopsis* will help scientists understand the molecular basis of plant growth and development and address fundamental questions in plant physiology, biochemistry, cell biology, and pathology.

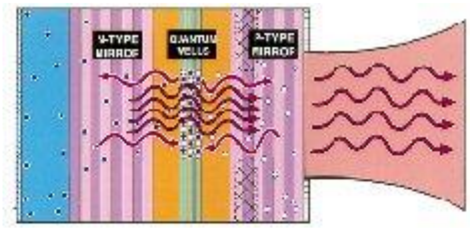
Scientific Impact: The MSU effort was instrumental in establishing *Arabidopsis* as a model organism for identifying and studying plant genes at the molecular level. Since the early sequencing of ESTs, studies using *Arabidopsis* have yielded many significant advances, including the discovery of plant hormone and signal receptor action and components of disease resistance.

Social Impact: Concentrated research on this single plant will provide detailed information that can be applied to a wide range of plant attributes relevant to energy, manufacturing, the environment, agriculture, and even human health. One result has been crops that are more resistant to the cold; further insights will help scientists make other plants easier to grow under adverse conditions, healthier to eat, and more disease resistant.

Reference: *Arabidopsis thaliana* Genome Sequencing Completed," *Nature*, December 14, 2000.

SC-Funding Office: Office of Basic Energy Sciences

2.23 New Opto-electronic Materials and Devices



Vertical Cavity Surface-Emitting Laser (VCSEL) (sideview). It is a sandwich of high tech materials that traps and uses electric current to generate a laser beam.

Stacks of ultrathin layers—each less than one-thousandth the thickness of a human hair—are the secret to a class of artificially grown materials that have enabled numerous advances in technology over the past generation. In 1981, scientists at Sandia National Laboratories were the first to predict the unique electronic and optical properties of strained-layer semiconductor (SLS) superlattices, and, a few years later, the first to make devices from them. These crystalline materials got their name because the spacing between the atoms in different layers is mismatched initially, but the thinness of the layers allows alignment by elastic strain without causing dislocations or other defects. Because the number, composition, and thickness of the layers can be varied over wide limits, scientists can tailor the electrical and optical properties to design materials and devices with targeted properties. This work has won a number of awards, including the American Physical Society's International Prize for New Materials in 1993.

Scientific Impact: This work established new areas of materials science and electronics as well as new research technologies; for instance, SLS materials are used to make transistors for high-frequency, low-noise electronic amplifiers, such as those found in radiotelescopes. These materials made it possible for scientists to tailor the wavelength (or color) of light-emitting devices (such as light-emitting diodes) and increase the speed of electrons in transistors.

Social Impact: The SLS technology revolutionized the multibillion-dollar field of opto-electronics and is a key to wireless communications. These materials enhance the performance and efficiency of semiconductor lasers and make possible new types of lasers with applications in optical communications, supermarket scanners, remote sensing, and medical diagnostics.

Reference: "Laser Gain and Threshold Properties in Compressive-Strained and Lattice-Matched GaInNAs/GaAs Quantum Wells", W. W. Chow, E. D. Jones, *Appl. Phys. Lett* 75, pp. 2891-93 (1999).

"Pressure Dependence of the Bandgap Energy and the Conduction-Band Mass for an N-Type InGaAs/GaAs Single-Strained Quantum Well", E. D. Jones, S. W. Tozer, and T. Schmiedel, *Physica E* 2, pp. 146-150 (1998).

"Study of Cyclotron Resonance and Magneto-Photoluminescence of N-Type Modulation-Doped In GaAs Quantum Well Layers and Their Characterizations", N. Kotera, E. D. Jones, K. Tanaka, H. Arimoto, M. Ohno, N. Miura, T. Mishima, edited by S. C. Shen, D. Y. Tang, G. Z. Zheng, and G. Bauer (*World Scientific*, Singapore, 199) pp. 591-598.

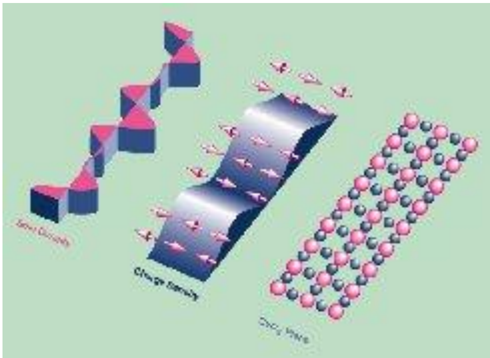
"Room-Temperature Continuous Wave InGaAsN Quantum Well Vertical-Cavity Lasers Emitting at 1.3 Microns", K. D. Choquette, J. F. Klem, A. J. Fischer, O. Blum, A. A. Allerman, I. J. Fritz, S. R. Kurtz, W.G. Breiland, R. Sieg, K. M. *Electronics Letters* Vol. 36, 1388 (2000).

"GaAsSb/InGaAs Type-II Quantum Wells for Long-Wavelength Lasers on GaAs Substrates", J. F. Klem, O. Blum, S. R. Kurtz, I. J. Fritz, and K. D. Choquette, *J. Vac. Sci. Technol*. B, Vol. 18, 1605 (2000). "Strained-layer semconductor superlattices from lattice mismatched materials." Osbourn, J.C. *J. Applied Physics* (53) p1586 (1982).

"InGaAs strained-layer semiconductor superlattices: A proposal for useful new electronic materials." Osbourn, J.C. *Phy Rev. B.* (27) p5126 (1983).

SC-Funding Office: Office of Basic Energy Sciences

2.24 Unraveling the Mystery of High-Temperature Superconductivity



Stripe Formation. Picture of the spin and charge densities in the copper-oxygen planes where the conducting electrons are located. Lower density antiferromagnetic regions are seen to alternate with higher charge density regions. Such an effect is far more probable in two dimensional, i.e., planar, geometrical arrangements.

Since the discovery in the 1980s of high-temperature superconductors, the Office of Science has supported research designed to explain and improve the physical behavior of these materials and develop methods of making wires and other objects from them. These materials conduct electricity with virtually no resistance at temperatures high enough to be cooled by liquid nitrogen (-196 degrees C, or -321 degrees F) instead of more costly helium. Studies at various national laboratories have led to discoveries concerning, for example, the relationships between magnetic behavior and superconductivity, and between material layering and current-carrying capability. Argonne National Laboratory clarified the nature of several different phases of vortex matter (compounds often break down at the vortex, where the molecules of different materials meet), leading to new configurations that improve conductivity. Argonne also built the first superconducting motor and developed a process for welding lengths of wire in a way that maintains superconductivity. Other investigators have observed "charge stripes" in materials exhibiting colossal magnetoresistance, an unusual and powerful effect that may be exploited in future magnetic recording devices. Years of research at Oak Ridge National Laboratory led to the development of processes that may enable the manufacture of long lengths of superconducting wires and tape.

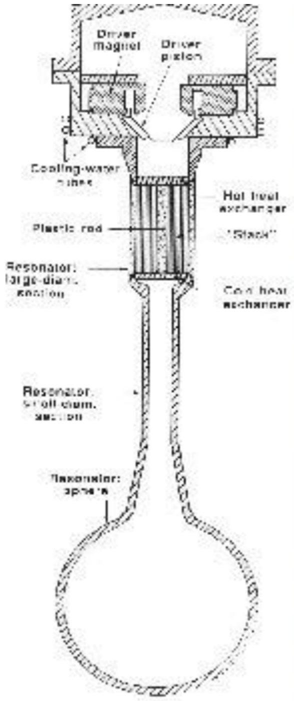
Scientific Impact: This research has greatly increased scientific understanding of high-temperature superconductors. As yet, there is no comprehensive theory that explains all of the experimental phenomena; this remains a key question in condensed matter physics.

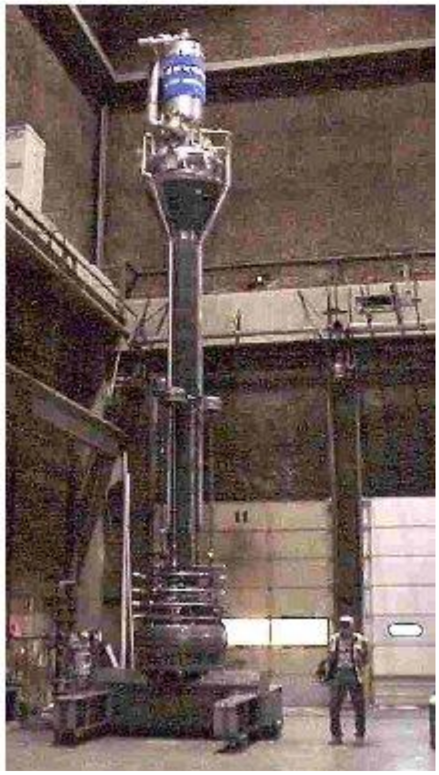
Social Impact: Superconducting wires and tape can carry 100 to 200 times more electric current than conventional wires. These innovations could enable the widespread commercialization of more efficient types of power generation, transmission, and electrical equipment and devices, offering tremendous energy savings and emissions reductions.

Reference: S.L. Bud'ko, G. Lapertot, C. Petrovic, C.E. Cunningham, N. anderson, and P.C. Canfield. "Boron Isotope Effect in Superconducting MgB2," *Physical Review Letters*, February 26, 2001.

SC-Funding Office: Office of Basic Energy Sciences

2.25 Harnessing the "Thermoacoustic" Effect





Thermoacoustic Refrigeration

A sound wave consists of oscillations in pressure, temperature, and displacement. Although the temperature oscillations are small, research during the past two decades has shown that this "thermoacoustic" effect can be harnessed to produce powerful, reasonably efficient heat engines, including heat pumps, and refrigerators. Thermoacoustic engines typically have no moving parts; at most, there is a single oscillating part (such as a loudspeaker) with no sliding seals. Thus, these engines have the potential to be both simple and reliable. Research by Greg Swift at Los Alamos National Laboratory on the thermodynamics of the thermoacoustic process has led to the development of prototype refrigerators with cooling powers up to tens of watts, and prototype engines with efficiencies approaching those of conventional engines. The research has spawned collaborative efforts that have resulted in advances in the theory, design, and construction of thermoacoustic devices.

Scientific Impact: Los Alamos' leadership in both the scientific and technological aspects of thermoacoustics since the mid-1980s has generated a sizeable academic research community around the world. The first international workshop on thermoacoustics will be held in 2001.

Social Impact: Thermoacoustic energy conversion (including conversion of heat to acoustic power, acoustic power to refrigeration, and acoustic power to mixture separation) is reasonably efficient and should be inexpensive and reliable in mass production. Efforts are under way to develop a natural-gas liquefier for use in remote locations, a residential co-generation system to produce both electricity and gas heat, an electric generator for deep-space probes, and a water chiller for use on submarines.

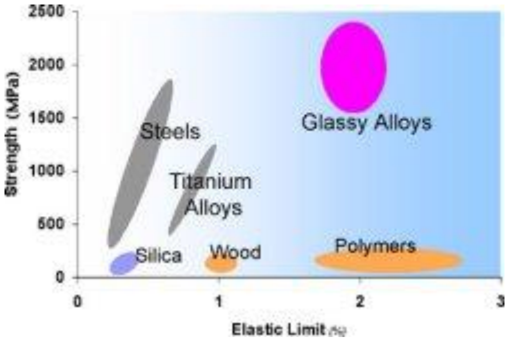
Reference: S. Backhaus and G.W. Swift. "A thermoacoustic-Stirling heat engine." *Nature*, 399:335-338, 1999.

G. W. Swift. "Thermoacoustic engines and refrigerators." *Physics Today*, pages 22-28, July 1995.

G. W. Swift. "Thermoacoustic engines." *J. Acoust. Soc. Am.*, 84:1145-1180, 1988.

SC-Funding Office: Office of Basic Energy Sciences

2.26 Metallic Glasses with Extraordinary Properties



Typical strengths and elastic limits for various materials. Metallic glasses are unique.

Metallic glasses with extraordinary magnetic properties, and practical methods for processing these materials, have been developed over the past four decades with support from the Office of Science and predecessor agencies. Pol Duwez at the California Institute of Technology produced the first ribbons of metallic glasses, which had unusual mechanical strength, magnetic behavior, and resistance to wear and corrosion that set them apart from conventional crystalline materials. The processing method involved chilling molten metal at rates in excess of 1,000,000 degrees C per second. Duwez and his student William L. Johnson also discovered other alloys that could be made into metallic glasses for high-efficiency magnets, but expensive processing was required to fabricate forms useful for motors and transformers. During the 1980s, Johnson developed new compositions that could be processed without rapid cooling in bulk or three-dimensional form (bulk forms are more than 20 times thicker than the roughly 40-micrometer ribbons), suitable for casting or possibly molding into complex shapes for precision parts, without the costs or wastes associated with machining. Recently, scientists at Los Alamos National Laboratory produced a bulk ferromagnetic glass with a record-low magnetic energy loss that does not require expensive processing, a form appropriate for energy conversion devices.

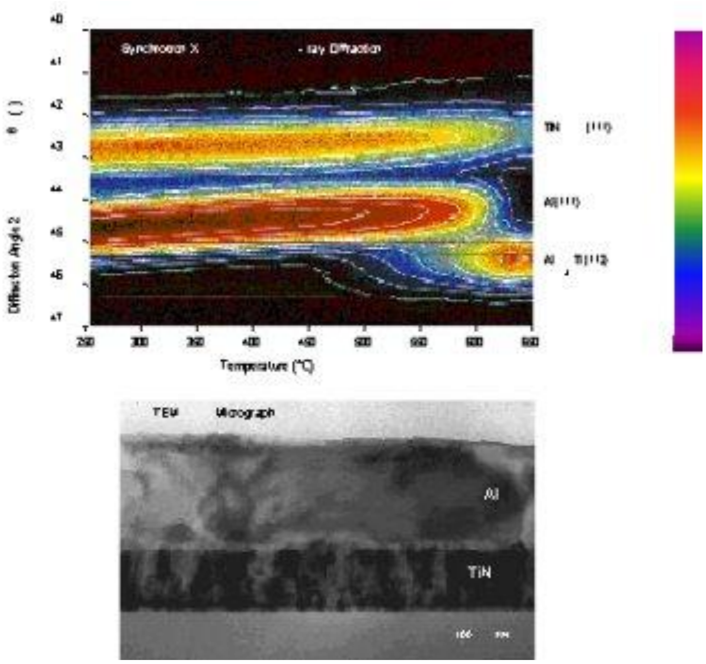
Scientific Impact: This research opened up a new area of materials science and technology—for which DOE was the sole U.S. supporter until recently—that offers opportunities for increasing the efficiency of magnets, motors, and transformers. Los Alamos is a world leader in research on bulk ferromagnetic glasses, the only form appropriate for motors and transformers.

Social Impact: These materials are used in products ranging from motor components to golf clubs and also have great potential for military applications. The use of bulk ferromagnetic glasses in energy-conversion devices would reduce costly losses from power-distribution systems and corrosion damage, and the consequent reduced use of energy from fossil sources would reduce the rate of release of carbon dioxide into the atmosphere.

Reference: Masuhr A, Busch R, Johnson WL. "Rheometry and Crystallization of Bulk Metallic Glass Forming Alloys at High Temperatures." *ISMANAM 1997 - Materials Science Forum*. Barcelona, Spain. Switzerland: Trans Tech Publications, 1998: 779-84.

SC-Funding Office: Office of Basic Energy Sciences

2.27 Extending the Science of Transition Metal Nitrides



Advanced Nitrides by Design. Synchrotron XRD and TEM microanalyses were used to determine interfacial reaction paths and mechanisms. The results allowed functional design of dramatically improved diffusion barriers.

Novel semiconductors, superconductors, and corrosion-resistant materials have been developed recently through nanoscale research on transition metal nitrides. J. E. Greene, I. Petrov, and colleagues at the University of Illinois Seitz Materials Research Laboratory, with Office of Science support, combined theoretical modeling with fundamental growth and characterization experiments to improve the basic mechanical and electrical properties of nitrides. They developed new processes for depositing these materials with control of atomic-scale reaction and diffusion, thereby designing whole families of alloys with unique properties that are impossible to achieve under equilibrium conditions. To achieve these properties, it was necessary to control grain size and texture on a scale on the order of 10 nanometers (nm), and to achieve interfacial widths of 0.1 nm to 1.0 nm. This work has many applications and has been recognized by many awards, including the 1999 David Turnbull Lectureship of the Materials Research Society, the 1998 David Adler Prize from the American Physical Society, and the Tage Erlanger Prize in Physics (the second-ranking Swedish prize in science after the Nobel Prize).

Scientific Impact: This work extended the science of transition metal nitrides, making possible the design of entirely new materials. These achievements also demonstrate the value of research on the nanoscale, an emerging field of great importance.

Social Impact: Transition metal nitrides already have practical uses; titanium aluminum nitride, for example, has become ubiquitous in wear-, corrosion-, and diffusion-resistant coatings for products such as cutting tools. The new alloys have enabled the use of copper interconnects in integrated circuits through the creation of improved diffusion barriers, thus paving the way for a new generation of faster computer chips.

Reference: J. S. Chun, I. Petrov, and J.E. Greene, "Dense fully 111-textured TiN diffusion barriers: Enhanced lifetime through microstructure control during layer growth" *J. Appl. Phys.*, 86 3633 (1999).

D. Gall, I. Petrov, P. Desjardins, and J.E. Greene, "Microstructural evolution and Poisson ratio of epitaxial ScN grown on TiN(001)/MgO(001) by ultrahigh vacuum reactive magnetron sputter deposition" *J. Appl. Phys.*, 86 5524 (1999).

SC-Funding Office: Office of Basic Energy Sciences

2.28 A New Type of Microscopy

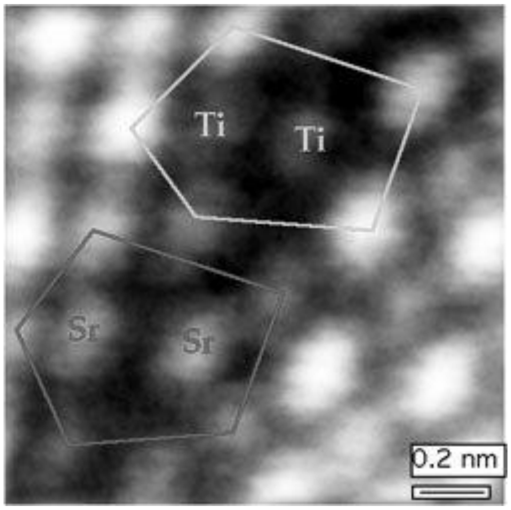


Image of a strontium titanate grain boundary taken with Z-contrast TEM.

A microscope invented with Office of Science support is the first technique to produce a direct image of a complex atomic structure while also identifying the atoms involved. Steve Pennycook of Oak Ridge National Laboratory combined elements of three existing electron microscopes to make the Z-contrast microscope, which uses electrons bounced off (scattered from) a sample to form an image of the atoms. Because the scattered intensity depends on the atomic number (Z) of the chemical element being probed, the image intensity provides a means of identifying the atoms. The method improves on scanning electron microscopes (which produce clear images but cannot penetrate materials), transmission electron microscopes (which produces images that cannot be interpreted directly as atomic structure), and the hybrid scanning transmission electron microscope (which produces outstanding microanalysis but poor-quality images). Z-contrast microscopy is particularly suited to the viewing of interfaces, grain boundaries, and defects in materials-features that cannot be analyzed well using indirect means. The Z-contrast microscope won an R&D 100 award from R&D Magazine as a significant new technology. Pennycook also received the Materials Research Society Medal and the Kurt J. Heinrich Award of the Microbeam Analysis Society.

Scientific Impact: Z-contrast microscopy has had major impact on the study of materials structure. It has achieved the highest resolution of a crystal structure ever recorded in a microscope and provided new information on the atomic-scale structure and chemistry of a variety of materials—correcting previously published quasicrystal structures, for example.

Social Impact: Z-contrast microscopes are commercially manufactured. This tool is likely to lead to dramatic advances in structural materials, superconductors, and semiconductors, especially in the smoothness of interfaces where different materials join, and thereby pave the way for improved computers, fiber-optic communications, medical imaging, and laser-disc players.

Reference: M. F. Chisholm and S. J. Pennycook, "Z-Contrast Imaging of Grain-Boundary Core Structures in Semiconductors," *MRS Bulletin* 22, 53 (1997).

SC-Funding Office: Office of Basic Energy Sciences

3 HIGH ENERGY AND NUCLEAR PHYSICS

3.1 First Evidence of a Third Family of Fundamental Particles

Professor Martin Perl, discoverer of tau lepton.

The third family of fundamental particles of matter became more than just a theory during the 1970s, when a series of experiments at the Stanford Linear Accelerator Center led to discovery of the tau lepton. The tau was the first actual evidence of the third generation of quarks (the smallest particles of matter), leptons (weakly interacting particles), and their anti-particles. For this discovery, Martin L. Perl won the 1995 Nobel Prize in Physics, sharing the honor with Frederick Reines (the discoverer, much earlier while at Los Alamos National Laboratory, of a particle in the first family). Perl's early experiments failed, until a new particle collider gave him access to a previously inaccessible region of energy, about 5 billion electron volts. The higher the energy levels in a particle collider, the smaller the structures that can be probed. Even then, years of observations involving tens of thousands of pieces of data were needed before the researchers were certain they had discovered a new lepton. The final identification of the tau as a lepton was achieved by measuring its lifetime with the vertex detector method, an important technique that was new at the time.

Scientific Impact: Evidence of the third family of fundamental particles inspired confidence in the Standard Model, the theory then being developed by physicists to explain matter and the forces of nature. The vertex detector method has been used to measure the lifetime of other fundamental particles and is now used universally to measure particle properties.

Social Impact: These studies answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "Properties of the Proposed Charged Tau Lepton," M. L. Perl et al., *Phys. Lett.* 70B: 487 (1977).

"Measurement of the Tau Lifetime," G. J. Feldman et al., *Phys. Rev. Lett.* 48: 66-69 (1982).

"Precise Measurement of the Tau Lifetime," J. A. Jaros, et al. *Phys. Rev. Lett.* 51: 955-958 (1983).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.2 Discovery of One of the Smallest Particles of Matter

The vertex detector used in this experiment at the Stanford Linear Collider.

Forces of nature are mediated by the interaction or exchange of particles called bosons. In 1989, experiments at Stanford Linear Accelerator Center and the European Laboratory for Particle Physics (also known as CERN) made precise measurements of the lifetime of the Z0 boson, which carries the "weak force" that allows particles to change form. The experiment was significant because it implied that only three families of fundamental particles exist. That's because the Z0 boson is short-lived and decays to certain other particles; the number of these particles influences the decay process. Precise measurement of the Z0 boson lifetime revealed that only three particles called neutrinos are produced. (If additional neutrinos were involved, then the Z0 boson would have additional ways to decay and thus a shorter lifetime than was indicated by the experiment.) This conclusion, which was supported by other studies, implies that only three families of matter exist. All three families have now been observed.

Scientific Impact: This work placed a firm cap on the possible complexity of the universe, at the level of its fundamental constituents. The results agreed with the Standard Model, physicists' current understanding of matter and the forces of nature.

Social Impact: These studies answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "First Evidence That the Number of Light Neutrinos = 3," G. S. Abrams et al., *Phys. Rev. Lett.* 63: 2173 (1989).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.3 A Limit on the Complexity of the Universe

The vertex detector used in this experiment at the Stanford Linear Collider.

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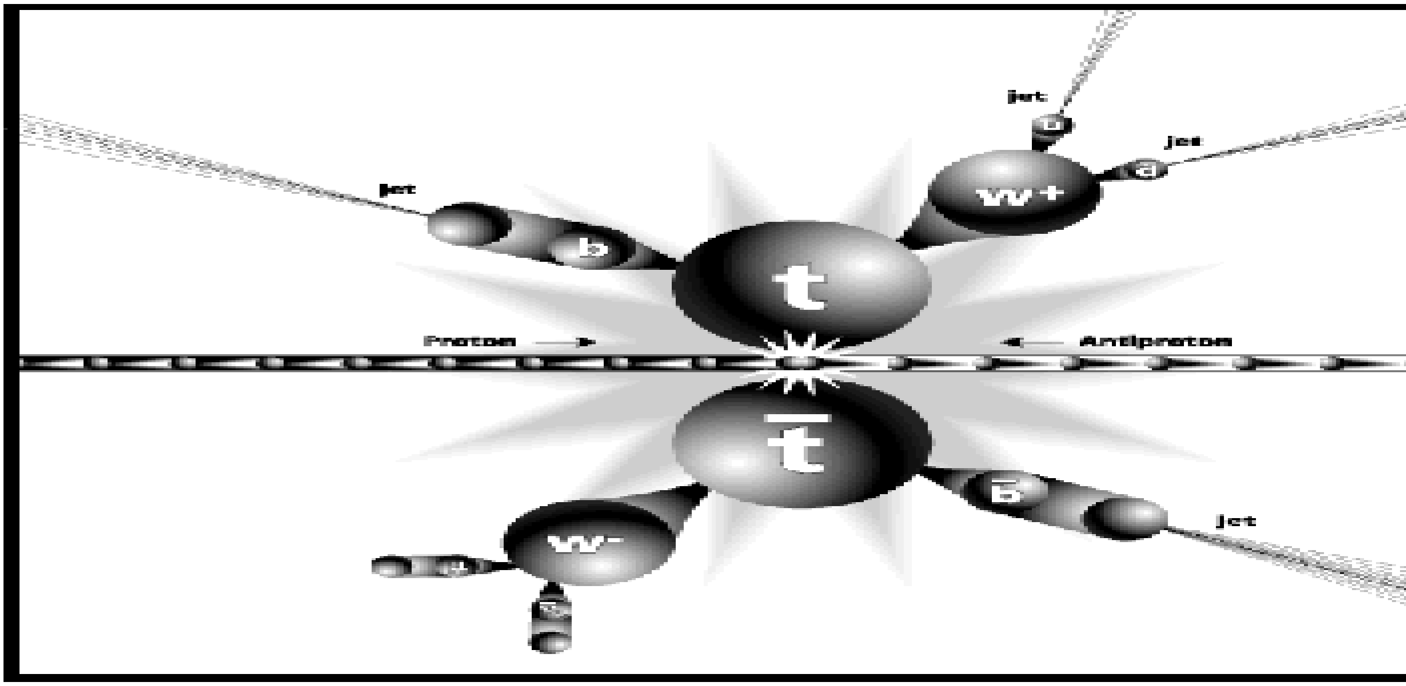
Reference: "First Evidence That the Number of Light Neutrinos = 3," G. S. Abrams et al., *Phys. Rev. Lett.* 63: 2173 (1989).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.4 Completion of the Third Generation of Matter



Colliding proton and antiproton produces top quarks.

Thanks to two recent discoveries at Fermi National Accelerator Laboratory, the third family of fundamental constituents of matter has been completed. In 1995, two experiments discovered the "top" quark, the last undiscovered quark of the six predicted to exist by current theory. Quarks are the smallest particles of matter; the top quark is the heaviest elementary particle known. Scientists worldwide had been seeking the top quark since 1977, when the third family's "bottom" quark was discovered at Fermilab. An experiment in 2000 found the elusive tau neutrino, completing the third generation of leptons (weakly interacting particles). Scientists were convinced it existed, but no one before had directly observed this near-massless particle, which barely interacts with surrounding matter. The team used elaborate equipment-including very strong magnets to remove all charged particles and 15 meters of shielding to remove all else but neutrinos-and spent three years looking for the neutrino's tracks, found in just four of 6 million potential interactions. The three families of quarks and leptons, together with forces that govern their interactions, make up the Standard Model of particle physics. The only missing piece now is the Higgs boson, the expected source of mass.

Scientific Impact: These discoveries required more than 30 years of technological advances and confirmed the value of equipment such as the Tevatron, the world’s highest-energy particle accelerator. Discovery of the tau neutrino also opened a door to studies of the connections among neutrinos and whether neutrinos have mass.

Social Impact: This confirmation of existing theory contributed to science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "Observation of the Top Quark," F. Abe et al., *Phys. Rev. Lett.* 74: 2626 (1995).

"Observation of the Top Quark," S. Abachi et al., *Phys. Rev. Lett.* 74: 2632 (1995).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.5 Confirmation of the Unification of Two Fundamental Forces

Professor Charles Prescott

Fundamental forces of nature include the electromagnetic force, which involves interaction between particle charges; and the weak force, which causes radioactive beta decay and is key to solar energy production, making possible the evolution of life on Earth. Once thought to be separate, these forces were unified in the electroweak theory, an important part of the Standard Model, physicists' current theory of matter and the forces of nature. In 1978, scientists at Stanford Linear Accelerator Center studied the scattering of high-energy electrons on deuterium nuclei and observed an effect attributable to a direct interplay between the electromagnetic and weak parts of the unified interaction. The results confirmed earlier predictions of unification by three scientists who shared the 1979 Nobel Prize in Physics for developing the electroweak theory. Among other things, the theory predicts a new type of weak interaction, in which the charges of reacting particles do not change—unlike the process of beta decay and similar to electromagnetic interactions.

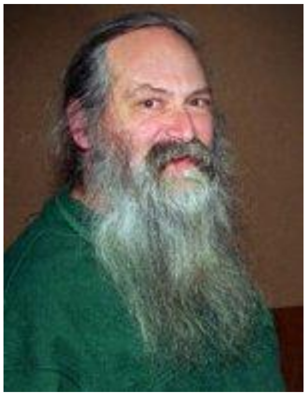
Scientific Impact: This work showed that the force responsible for radioactivity is closely related to that responsible for binding atoms together and producing light and electricity. The Stanford experiment was cited in the Nobel literature as important confirmation of the unified electroweak interaction, a theory that contributed to the intense development of particle physics in the 1970s.

Social Impact: Research on the forces of nature helps explain the workings and history of the universe, extending human understanding of the environment and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "Confirmation of Weak Neutral Currents," C. Y. Prescott et al., *Phys. Lett.* 77B: 347 (1978).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.6 Methods for Complex Calculations



Dr. Michael Creutz

Quarks are tiny particles, but a force like the weight of 14 tons binds them together. That's one of the findings of physicists investigating quantum chromodynamics (QCD), the theory describing the "strong force" that binds subnuclear particles called quarks and gluons. The Office of Science has supported the development of various computer-based techniques for performing the difficult calculations of QCD. Theorists at Brookhaven National Laboratory, Fermi National Accelerator Laboratory, and elsewhere have made relevant calculations. Michael Creutz of Brookhaven demonstrated that properties of QCD could be computed numerically using a lattice of discrete points of time and space instead of a continuum. Creutz provided strong evidence that quarks cannot be isolated (the force between quarks does not decrease, even as they are moved farther apart), thus mathematically confirming QCD. He won the American Physical Society's Aneesur Rahman Prize for Computational Physics in 2000. Another project involving Columbia University, Brookhaven, and the Riken Institute produced the world's fastest multipurpose, noncommercial supercomputer. The computer turns space and time into a four-dimensional lattice (or a three-dimensional grid for any moment in time) and enables scientists to calculate interactions between quarks at larger distances than possible with other methods. The "do it yourself" approach to construction limited costs to about $1.8 million for the entire project and won the 1998 Gordon Bell Award for most cost-effective computing.

Scientific Impact: Creutz's methods have been applied to various theoretical problems in physics; lattice calculations are the best estimates for the temperature of the elusive quark-gluon plasma, a form of matter dating back to the Big Bang creation of the universe. The Brookhaven supercomputer's speed will enable scientists to simulate and predict the behavior of such subatomic particles and phenomena.

Social Impact: The supercomputer project has led to affordable teraflop-scale (1 thousand billion calculations per second) computing engines. Algorithms developed for QCD computations have potential applications in superconductivity, development of magnetic materials, and other fields of commercial interest.

Reference: "Monte Carlo study of quantized SU(2) gauge theory," M. Creutz, *Phys. Rev.* D21, 2308-2315 (1980).

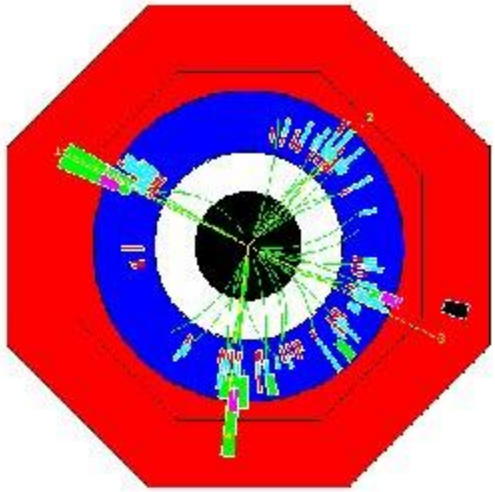
Quarks, Gluons, and Lattices, M. Creutz (Cambridge Univ. Press, 1983).

Nuclear Physics B—Proceedings Supplements, Volume 83-84 (2000).

Proceedings of the XVIIth International Symposium on Lattice Field Theory, Pisa, Italy, 29 June 1999.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.7 Zeroing in on the Elusive Higgs Boson



SLD Event Display of a Z particle decaying to two quarks. An electron and positron travelling in opposite directions (perpendicular to this page) collided at the center of the detector and annihilated, creating a Z. The Z subsequently decayed to a quark and anti-quark, which then hadronized to form two jets of particles traveling in opposite directions. These are the two jets of green tracks seen in this projection.

Research supported by the Office of Science is making progress in the intense search for the Higgs boson, which may be the force that finally explains why some fundamental particles have mass, but others do not. Higgs is the last undiscovered component of the Standard Model, physicists' current theory of matter and the forces of nature. The model includes three families of particles called quarks and leptons; bosons carry forces between other particles. The Standard Model predicts a relationship between the masses of the Higgs boson, the W boson (which carries the "weak force"), and a particle called the top quark. Precise measurements of the properties of the top quark and W boson at Fermi National Accelerator Laboratory and the Zo at the Stanford Linear Accelerator Center in the 1990s significantly narrowed the predicted range for the mass of the Higgs boson. The SLAC experiments obtained what remains the most precise prediction of the mass of the Higgs, hinting that it should be light.

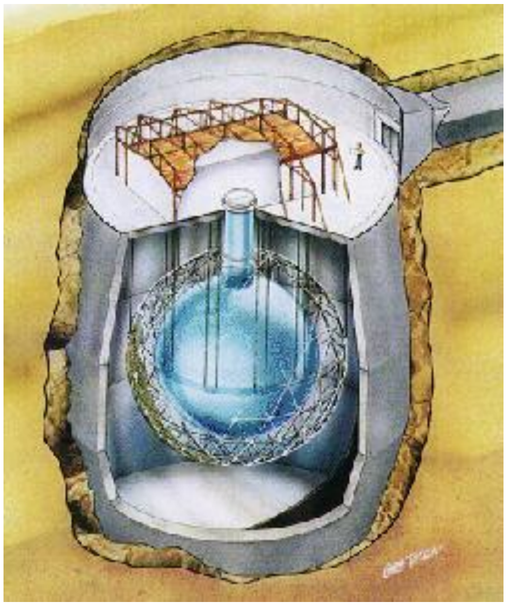
Scientific Impact: These experiments told scientists what mass range to seek in direct measurements of the Higgs boson; when the Higgs is found, comparisons of direct and indirect measurements will provide a strong test of the Standard Model. The results also suggest that the Higgs might be within reach of existing accelerators.

Social Impact: Research on subatomic particles answers questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "Improved Direct Measurement of Leptonic Couplings Asymmetries with Polarized Z Bosons," K. Abe et al. (The SLD Collaboration), *Phys. Rev. Lett.* 86, 1162, (2001).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.8 The Missing Solar Neutrinos



Sudbury Neutrino Observatory in Canada

A neutrino is created, along with an electron, when the nucleus of an atom disintegrates through beta decay. Neutrinos are produced, for example, in the nuclear reactions that fuel the burning of stars, such as the Sun. But for some reason, fewer electron neutrinos reach the Earth than would be expected based on known solar processes. This phenomenon was first suggested by observations at the oldest solar neutrino detector (in South Dakota), for which Raymond Davis of Brookhaven National Laboratory won the 2000 Wolf Prize, and a detector in Japan. The results were confirmed in the 1990s by precise radiochemical experiments called SAGE and GALLEX, supported by the Office of Science. These experiments differ in design from the previous two and detect neutrinos of different energy levels. SAGE and GALLEX also stimulated searches for neutron oscillations (conversion from one type to another), because solar neutrinos may change as they journey from the Sun to the Earth. The search for the missing solar neutrinos continues, led by Sudbury Neutrino Observatory in Canada in an effort that involves several national laboratories, and another group in Japan (also involving Americans).

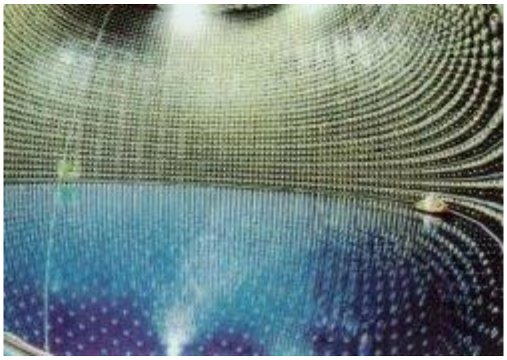
Scientific Impact: Studies of neutrinos have significant effects on theories in physics, astronomy, and cosmology. Because of these experiments, many physicists and astronomers now believe that the missing neutrinos are due not to a faulty understanding of how the Sun works, but rather to an overly simplistic view of neutrino behavior.

Social Impact: Research on solar neutrinos could be the key to finding the Holy Grail of physics, the so-called unified theory that goes beyond the present Standard Model in explaining matter and the forces of nature. Thus, this research may lead to new understanding of the universe and the place of humans in it.

Reference: "Solar Neutrino Experiments: The Next Generation," Bahcall et al., *Physics Today* July: p. 30 (1996).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.9 Evidence for Neutrino Mass



The Super-Kamiokande detector, half-filled with pure water. (Courtesy of the Institute for Cosmic Ray Research, the University of Tokyo.)

For many years, scientists believed that neutrinos, released with electrons when a nucleus undergoes beta decay, might be massless. But in 1995, after collecting three years of data, Los Alamos National Laboratory reported evidence for neutrino oscillations, or transformations of one type of neutrino into another. This finding was supported recently when an international team, including Americans, working at Japan's Super-Kamiokande detector (supported in part by the Office of Science) demonstrated that the muon type of neutrinos oscillate, probably changing into the tau type, as they pass through the Earth. Such oscillations can occur only if neutrinos have mass, albeit the smallest yet observed for elementary particles, and there is "mixing" among certain particles—phenomena that contradict the Standard Model, physicists' current theory of matter and the forces of nature. The difference in mass of the two types of neutrinos was measured based on energy and flight distance from neutrino production in the atmosphere by cosmic radiation to an underground instrument.

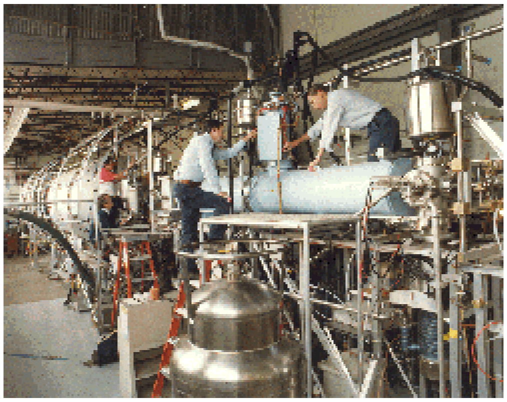
Scientific Impact: When verified, this discovery will force a revision in the Standard Model. Furthermore, scientists might have some help in answering a question posed by current models of the universe, which suggest that more matter is present than can be detected by observing electromagnetic radiation; neutrinos might constitute the missing "dark matter."

Social Impact: This discovery, because it may alter estimates of the total mass of the universe, has implications for human understanding of the origin and eventual fate of the universe. The measured neutrino mass is sufficient that the relic neutrinos made in huge numbers at the time of the Big Bang creation of the universe would account for much of its mass.

Reference: "Tau Neutrinos Favored over Sterile Neutrinos in Atmospheric Muon Neutrino Oscillations," The Super-Kamiokande Collaboration, *Phys. Rev. Lett.* 85: 3999-4003 (2000).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.10 Setting Limits on the Mass of the Electron Anti-Neutrino



The apparatus at Los Alamos used to set a limit on the mass of the electron antineutrino. The superconducting solenoid containing the gaseous tritium source is being examined by John Wilkerson (right) and Tom Bowles (center). In the background Hamish Robertson (left) and Mel Anaya are inside the cage of conductors used to cancel the Earth's magnetic field. Behind them is the high-resolution magnetic spectrometer.

Dr. R.G. Hamish Robertson

Neutrinos are created with electrons when the nucleus of an atom disintegrates through beta decay. Scientists know roughly how many neutrinos exist as leftovers from the Big Bang creation of the universe; however, their mass is a mystery. The mass range was narrowed in 1991, when scientists at Los Alamos National Laboratory announced a new top limit (9.3 electron volts, or eV) for the mass of the electron anti-neutrino (one type of neutrino), discovered through measurements of the beta decay of molecular tritium. From these data, the scientists determined that less than 30 percent (and consistent with zero) of the mass of the universe comes from electron anti-neutrinos, and thus, that they cannot constitute the bulk of the "dark matter" that makes up some 90 percent of the mass of the universe. Dark matter is nonluminous material that cannot be detected by observing electromagnetic radiation, but whose existence is inferred from current models of the universe. The electron anti-neutrino would need a mass exceeding 10 eV for it to constitute the primary form of dark matter. R. G. Hamish Robertson won the 1997 Tom W. Bonner Prize from the American Physical Society largely for this work.

Scientific Impact: Determining if dark matter exists, and in what quantity, is among the most challenging problems in modern astrophysics. This work is generally viewed as a textbook example of how to probe the nature of mass in the universe, and its success paved the way for improved experiments that have lowered the electron anti-neutrino mass limit to about 3 eV.

Social Impact: This experiment gives insight into the question of what the universe is made of thus, one possible explanation of what the universe is made of, thus contributing to human understanding of nature and improvements in science education. This finding also helped stimulate a worldwide research effort in neutrino physics that has brought scientists from many countries together to work on the same problem.

Reference: "Limit on Electron Antineutrino Mass from Observation of the b decay of Molecular Tritium," R. G. H. Robertson et al., *Phys. Rev. Lett.*, 67: 957 (1991).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.11 Beyond the Standard Model?

The world's largest superconducting magnet—the Muon Storage Ring at Brookhaven National Laboratory.

Quantum Electrodynamics (QED) describes how electrically charged particles and electromagnetic fields interact. First developed in the 1920s, the theory was revised and improved over the years until it seemed to agree with experimental results. But it was challenged in 2001, when a team led by Brookhaven National Laboratory conducted the most sensitive test yet of QED. The measurement of a key property (the anomalous magnetic moment) of the muon, a subatomic particle not found in ordinary matter, is a factor of 5.6 more precise than previous measurements and deviates from the value predicted by current theory. The scientists collected data from more than 1 billion muon decay events to measure the target property, which is among the most precisely known quantities in physics. The experiment showcased the latest research technology, including a very intense source of muons, the world's largest superconducting magnet, and very precise and sensitive detectors. The finding has yet to be verified; the Brookhaven data still are being analyzed, and QED was confirmed recently at Los Alamos National Laboratory, which made the most precise measurement ever of the hyperfine structure of muonium (composed of a muon and an electron), providing values for the muon mass and magnetic moment.

Scientific Impact: The Brookhaven work poses a direct challenge to the Standard Model, physicists' current overarching theory of matter and the forces of nature. The experiment may have revealed new physics, such as that described by supersymmetry theory, which predicts the existence of companion particles with unusual magnetic effects for all known particles.

Social Impact: Brookhaven's preliminary results, if supported and verified by additional analyses, would lead to new understanding of the physical world and associated improvements in science education.

Reference: H. N. Brown et al., *Phys. Rev. Lett*. 86, 2227 (2001).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.12 Unraveling the Mystery of Antimatter

Apparatus used to regenerate short-lived K mesons for the CP experiment.

Early in the evolution of the universe, matter and its mirror image, antimatter, were equally abundant; but today, antimatter is rare, for reasons not fully understood. A recent observation at Fermi National Accelerator Laboratory lessened the mystery somewhat. The 1999 experiment focused on mesons, short-lived pairings of a quark particle and the corresponding anti-quark. The researchers observed direct charge-parity (CP) violation in the decay of K mesons, or kaons, supporting the picture of CP violation provided in the Standard Model, physicists' current theory of matter and the forces of nature. The phenomenon of CP violation—which shows that matter and antimatter do not always behave symmetrically—was first discovered in kaon processes at Brookhaven National Laboratory in 1964, resulting in a 1980 Nobel Prize for Val Fitch and James Cronin. The definitive nature of the Fermilab result was dramatic and unexpected.

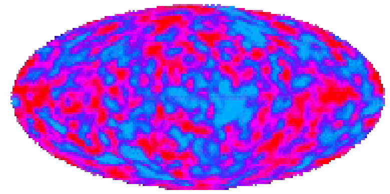
Scientific Impact: The result established the existence of direct CP violation beyond reasonable doubt and eliminated the long-standing hypothesis of a proposed "superweak" interaction as its source. This was a significant advance in understanding of the asymmetry in the behavior of matter and antimatter.

Social Impact: CP violation may be responsible for the survival of matter—including humans—and the disappearance of antimatter. Thus, this research extends human understanding of the origin and history of the universe and contributes to improvements in science education.

Reference: Phys. Rev. Lett. 83, 22 (1999). hep-ex/9905060.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.13 Detecting the Afterglow of the Big Bang



Anisotropy in the cosmic microwave background radiation.

Since 1964, when cosmic microwave background radiation was first discovered, scientists have searched the skies for evidence of temperature variations that might reflect the origins of the universe. In 1977, a team led by astrophysicist George Smoot of Lawrence Berkeley National Laboratory reported the first measurements of temperature variations in the microwave sky, but this irregularity was attributed to the motion of the Earth's galaxy in space. Smoot and colleagues already had begun developing a highly sensitive radiometer for detecting ancient microwaves, and it finally was launched aboard a satellite in 1989. Since then, Lawrence Berkeley scientists have used radiometers and powerful computers and algorithms to observe hot and cold ripples in the microwave radiation afterglow of the Big Bang. Today, this anisotropy is thought to be the primordial seed from which, over billions of years, the galaxies and large structures of the present-day universe grew.

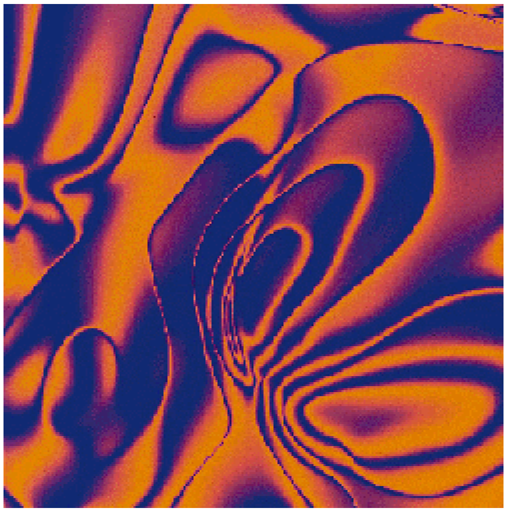
Scientific Impact: The temperature and size of the spots detected are in agreement with theories suggesting that up to 90 percent of the universe consists of mysterious "dark matter," the existence of which is inferred only because its gravity influences the motion of ordinary matter. Understanding of microwave background radiation, when combined with the eventual discovery of dark matter, will unify physics on the largest and smallest scales, fusing together the fields of cosmology and particle physics.

Social Impact: The patterns observed in microwave sky are like footprints left by the Earth's ancestors 15 billion years ago, only these footprints are gravitational effects. Thus, this work expands human understanding of how the universe evolved and contributes to science education.

Reference: "Structure in the COBE DMR First Year Maps," G.F. Smoot et al., *Astrophys. J.* 396:L1-L5 (1992).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.14 The Inflationary Universe



Energy distribution in an axion field.

The foundation of modern cosmology was laid in 1981, when physicist Alan Guth of the Massachusetts Institute of Technology developed an extension to the standard Big Bang model of the universe called the inflationary theory. This theory allows astronomers to trace the history of the universe back to a tiny fraction of a second after the Big Bang, when the strong, weak and electromagnetic forces identified by current theory were unified into a single electronuclear force. With Office of Science funding, Guth worked out the cosmological consequences of a phase transition in the universe, which in its earliest moments supercooled and then, in a fraction of a second, rapidly expanded exponentially, by many orders of magnitude. This model has been further developed by Andreas Linde of Stanford University, Paul Steinhardt of Princeton University, and others. Since the inflationary theory was proposed, other developments have emerged that may enable scientists to probe events occurring at an even earlier stage, perhaps even before the creation event itself.

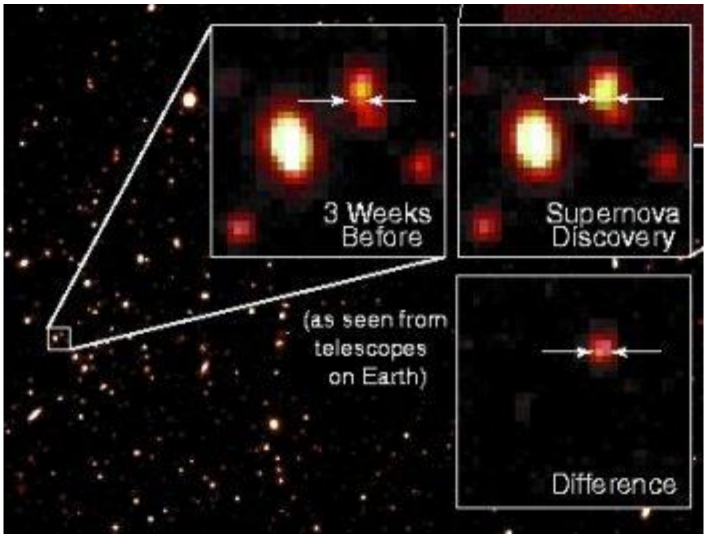
Scientific Impact: The inflationary theory solves many problems of standard Big Bang cosmology models, explaining, for example, why the universe appears so close to the transition between endless expansion and eventual contraction. The theory also suggests why the universe appears so homogeneous; at first it was so condensed that it became uniform, a condition well preserved by the very rapid expansion.

Social Impact: Widely accepted among theoretical physicists, the inflationary theory helps humans better understand nature and contributes to improvements in science education.

Reference: *Scientific American Presents* (ISSN 1048-0943), Volume 9, Number 1, 1998.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.15 Expansion of the Universe is Accelerating



Discovering a Supernova

Using a search technique that enables scientists to see violent explosions of dying stars "on demand," Saul Perlmutter of Lawrence Berkeley National Laboratory led a team to the surprising discovery that the expansion of the universe is accelerating, and thus is likely to continue doing so forever. The discovery was based on the identification and measurement during the 1990s of the most distant supernovas ever observed. Observations of rare type Ia supernovas—astronomical "standard candles" that all have the same intrinsic brightness—placed them much farther away than would be expected based on standard analyses of their emitted light. By comparing the distance to these exploding stars with the distance of their home galaxies, researchers calculated how fast the universe was expanding at different times in history. To ensure that supernovas were seen during limited telescope time, the team devised a strategy of imaging patches of sky just after a new moon, when the sky is dark, and then again three weeks later when supernovas show up as bright points of light. The discovery was selected by the journal Science as the top breakthrough of 1998.

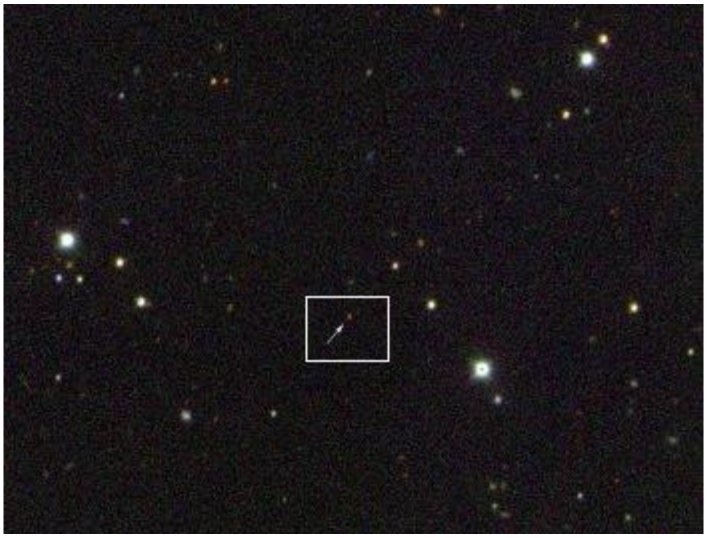
Scientific Impact: This work overturned the common assumption that the expansion of the universe was slowing down because of gravity. The results also provided strong evidence of a mysterious, self-repelling property of empty space—the cosmological constant first proposed by Albert Einstein—which may represent much of the total mass-energy density of the universe.

Social Impact: SOCIAL IMPACT: These findings raise profound questions about the ultimate fate of the universe and the Earth, with the promise of as-yet-unimagined impacts on human society.

Reference: S. Perlmutter et al. (1998), presentation at the January 1998 Meeting of the American Astronomical Society, Washington, D.C., LBL Report Number LBL-42230; referenced in B.A.A.S., Volume 29, page 1351 (1997); astro-ph/9812473; S. Perlmutter et al., *Astrophysical Journal*, 517: 565-586 (1999); astro-ph/9812133.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.16 The Most Distant Object Ever Observed



Most distant quasar—redshift 5 (the faint red dot at the arrow.)

An unassuming speck of red light assumed gargantuan proportions in 2000, when scientists at the Sloan Digital Sky Survey used detection and computational techniques borrowed from particle physics to find the most distant object ever observed. This quasar had the highest redshift ever seen, corresponding to a distance of 27 billion light years from Earth. Redshift (meaning the light appears shifted to the red end of the spectrum) is used as a measure of the distance of celestial objects. Because the universe is expanding, the quasar was only about 4 billion light years from Earth when the light seen now was emitted-at a time when the universe was very young, less than 1 billion years old. Quasars are compact, luminous objects believed to be the high-energy nuclei of young galaxies. Finding distant quasars is a specialty of the Sky Survey, launched in 2000 as the most ambitious astronomical survey ever. It will exceed all predecessors in scale, mapping in detail one-quarter of the entire sky and producing more sensitive and accurate images than ever made before by using electronic light detectors instead of photographic techniques. The project involves 11 universities and other institutions, including Fermi National Accelerator Laboratory. The telescopes are located in New Mexico.

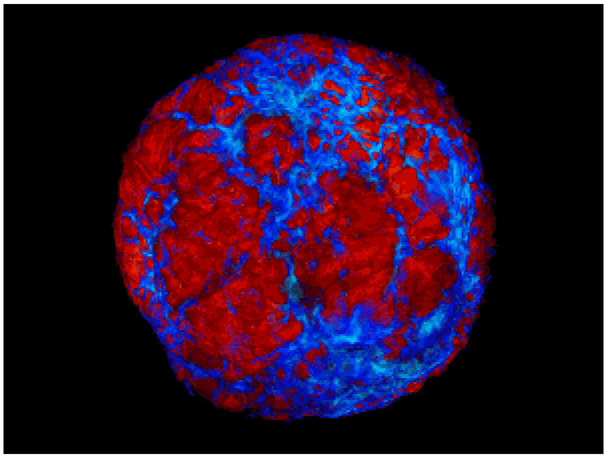
Scientific Impact: The Sky Survey is producing a field guide to the universe that will be used by scientists for decades to come. It will have a significant impact on astronomical studies ranging from the origin and evolution of galaxies to the properties and distribution of the dust from which stars like the sun were created.

Social Impact: The Sky Survey is extending the practice of mapmaking—laying the gridwork for reality—to cosmography, the science of mapping the universe and determining the place of humans in it. It will enhance 100-fold humans' three-dimensional picture of the universe, producing a quantity of information rivaling the content of the Library of Congress.

Reference: "The Discovery of a Luminous z=5.80 Quasar from the Sloan Digital Sky Survey," X. Fan et al., to be published in *Astron. Journal*.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.17 The Stars Above Us, Govern Our Conditions



Computer simulation of a Red Giant star.

The origins of chemical elements found on Earth-nuclear reactions that take place in stars—were discovered and confirmed by researchers supported by the Office of Science and predecessor agencies. The late William Fowler of the California Institute of Technology won half of the 1983 Nobel Prize in physics for his work in elucidating this process of nucleosynthesis. Fowler carried out experimental studies of nuclear reactions of astrophysical interest as well as theoretical calculations. During the 1950s, he and co-workers developed a complete theory of the formation of the chemical elements in the universe. (Their paper opens with the above quote from Shakespeare's King Lear.) An extensive series of neutron capture measurements performed at the Oak Ridge Electron Linear Accelerator since the 1970s further substantiated the theory. Other research conducted at national laboratories using reactions involving unstable nuclei also has contributed to understanding of the inner workings of astrophysical objects.

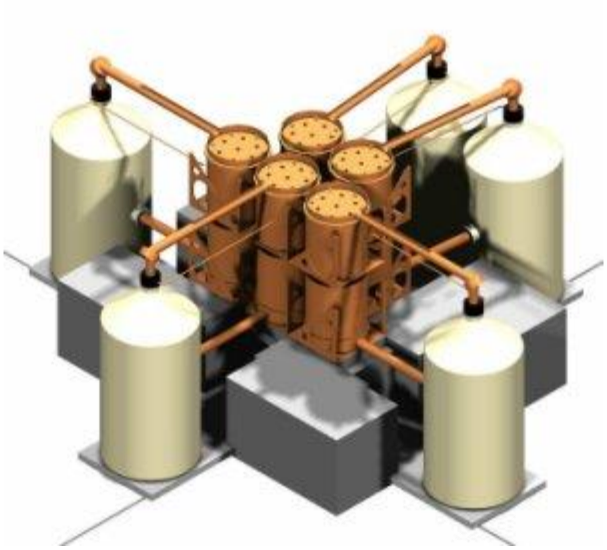
Scientific Impact: This work has yielded fundamental understanding of the chemical evolution of the galaxy and formation and age of the solar system. Fowler's theory remains the basis of knowledge in this field, and recent progress in nuclear physics and space research has further confirmed its correctness.

Social Impact: Scientists now know that half of the chemical elements heavier than iron were synthesized in Red Giant stars and dispersed throughout the galaxy as stardust blown by stellar winds. These elements are essential to human life; in other words, humans are made of stardust.

Reference: "Synthesis of the Elements in Stars," E. M. Burbidge et al., *Rev. Mod. Phys*. 29: 547 (1957).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.18 Rare Double Beta Decay Process is Observed



Complete Majorana Instrument, shielding removed.

A very rare form of nuclear disintegration called double beta decay was observed for the first time in 1986. This process, in which a nucleus emits two electrons and two antineutrinos, was observed in an isotope of selenium by Michael Moe and colleagues at the University of California, Irvine, with Office of Science support. Later, double beta decay was seen in other nuclei, including forms of calcium, germanium, and molybdenum. The methods developed for the experiment are being used to search for another rare decay mode, neutrino-less double beta decay, in which only the two electrons are emitted. This process could occur only if an electron neutrino is its own antiparticle and if neutrinos have mass, in violation of the Standard Model (physicists' current theory of matter and the forces of nature). Given the prevalence of neutrinos in the universe, even a tiny mass could account for much of the mysterious "dark matter" that emits no visible radiation but constitutes 90 percent of the mass of the universe.

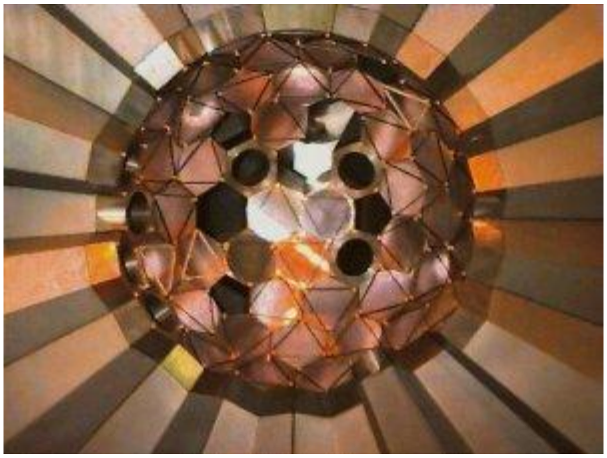
Scientific Impact: The measurement of the double beta decay rate provides key information that will be needed to determine neutrino mass once neutrino-less double beta decay is observed. In addition, the ultrasensitive techniques developed for these experiments are being used to search for other forms of dark matter.

Social Impact: Although research on double beta decay is new, single beta decay has many applications, including diagnostic and therapeutic medicine, and archeological dating. For example, doctors can examine functional images of patients' organs using positron emission tomography or treat thyroid disorders using a radioisotope of iodine, and carbon-14 dating is used to establish the age of ancient objects.

Reference: "Double Beta Decay," S. P. Rosen and Michael K. Moe, *Scientific American* November, 1989, p. 30.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.19 Unusual Nuclei May Answer Long-Standing Questions



Gammasphere is a very sensitive detector of gamma rays submitted from nuclei.

The core of an atom is the nucleus. Existing models of nuclear structure have been challenged recently by the discovery at several national laboratories of nuclei with extended shapes and other unusual characteristics. These properties were observed in nuclei at the extremes of excitation energy, angular momentum, deformation, and other parameters. For instance, superdeformed nuclei with a 2:1 axis ratio were found that spin very rapidly and exhibit identical gamma-ray decay properties. Other nuclei have a diffuse "halo" of loosely bound neutrons. These properties, found only in laboratories on Earth, may be important in the synthesis of heavier elements in giant and exploding stars. Evidence also has been found for superheavy nuclei, which may be the first indication of the long-sought "island of stability" beyond the previously known nuclei found in nature (i.e., uranium). These studies have been conducted at Argonne, Lawrence Berkeley, and Oak Ridge national laboratories.

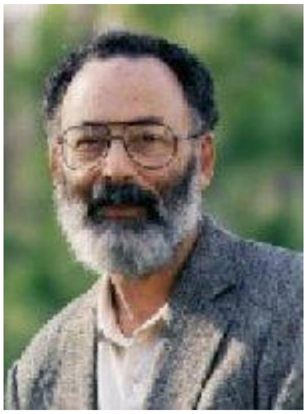
Scientific Impact: Studies of unstable isotopes (different forms of chemical elements) helps scientists understand the genesis of elements in stars and evolution of stellar systems. Nuclei with extended shapes and other properties near the extremes also test existing models and fundamental theories of the nucleus.

Social Impact: These studies help answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "Observation of a Discrete-Line Superdeformed Band up to 60 h in 152D," P.J. Twin et al., *Phys Rev. Lett.* 55: 1380 (1986); "Superdeformed Shapes at High Angular Momentum," P.J. Nolan and P.J. Twin, *Ann. Rev. Nucl. Part. Sci.* 38: 533-62 (1988); "Superdeformed Nuclei," R.V.F. Janssens and T-L. Khoo, *Ann. Rev. Nucl. Part. Sci*. 38 (1988).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.20 A Theory for Deducing Quark Behavior



Nathan Isgur

Physicists have difficulty studying individual quarks, because these smallest particles of matter are always bound together in pairs or groups of three. The heaviest of the six quarks found in nature have been the most baffling. But such studies are easier now, thanks to a method for understanding quarks developed in the early 1990s. "Heavy quark effective theory" enables physicists to deduce the individual behavior of one type of quark (the bottom quark) by showing how its properties can be directly inferred from measurements of another type (the charm quark). The six quarks identified in nature (in order of increasing mass) are distinguished by the terms up, down, strange, charm, bottom, and top. The heaviest (the top quark) is about 100,000 times the mass of the lightest (the up quark). The theory is based on seven years of theoretical work by Nathan Isgur of Thomas Jefferson National Laboratory and Mark Wise of California Institute of Technology, and a third researcher working independently.

Scientific Impact: This theory made it easier to study bottom quarks and pairs of them—important particles in ongoing studies of why the universe favors matter over its mirror image, antimatter. These papers also have generated thousands of other papers that offer new insight into another theory describing the "strong force" that binds subnuclear particles such as quarks.

Social Impact: These studies help answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: N. Isgur and M.B. Wise, *Phys. Lett.* B232, 113 (1989); 237, 527 (1990); *Heavy Quark Physics*, Aneesh V. Manohar, Mark B. Wise, Cambridge University Press (2000).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.21 The World's Most Powerful Accelerator

The superconducting Tevatron is the lower ring of magnets (the old main ring is above).

High-energy particle accelerators help explain many mysteries of matter, space, and time, enabling physicists to study the smallest objects ever found and recreate the conditions of the early universe. Fermi National Accelerator Laboratory's Tevatron, which accelerates and collides protons and antiprotons in a four-mile underground ring, is the most powerful accelerator in the world. It began operating in 1986, achieving collisions at energies of 1.6 trillion electron volts, about 1,600 times the rest mass of the proton. Among its innovations, the Tevatron pioneered the use of superconducting accelerator magnets, which, by generating increased magnetic fields with no resistive losses, help raise energy levels by keeping the speeding particles within the ring. The higher the energy levels in a particle collider, the smaller the structures that can be probed.

Scientific Impact: The Tevatron enables scientists to push the frontiers of both particle physics and cosmology. In 1995, research using this machine led to the discovery of the "top" quark, a fundamental constituent of matter. Superconducting accelerator magnets have become essential to many high-energy accelerators, both already built and planned for the future.

Social Impact: Particle collisions at the Tevatron give humans a way to see the smallest constituents of matter. Studies performed here expand human understanding of nature and contribute to improvements in science education.

Reference: "Initial Operation of the Tevatron Collider," Rolland Johnson, *Proceedings of the 1987 IEEE Particle Accelerator Conference* (87CH2387-9).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.22 First Linear Collider Offers New Possibilities

The SLAC Linear Collider (SLC)

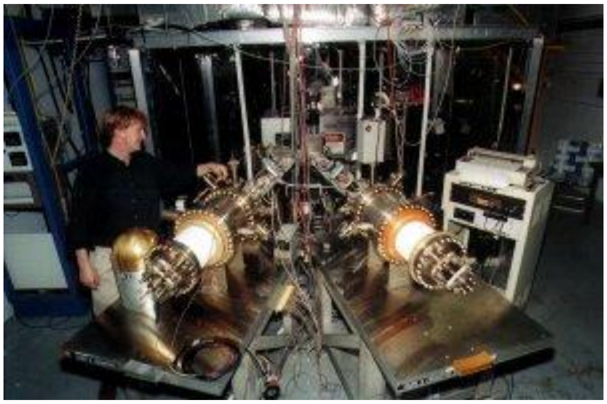
In 1989, the world's first linear collider, featuring beams of electrons and positrons (anti-electrons), began operating at Stanford Linear Accelerator Center. The SLAC Linear Collider (SLC) was based on new accelerator technology and offered the possibility of reaching higher-energy electron collisions in a more cost-effective manner than conventional ring designs. In 1998, the first "disruption enhancement" was achieved, in which beam density is high enough to cause the beams to shrink during the collision, an effect that doubles luminosity. Because of the high electron beam polarization and very small beam size at the collision point, SLC was able to make the world's most precise measurements of several key electroweak parameters—elements of the Standard Model, physicists' current understanding of matter and the forces of nature. Since then, a circular electron-positron collider has been built at the limit of energy possible for such a design. Operating at its highest energy, this machine may have seen evidence of the Higgs boson, the last missing piece of the Standard Model.

Scientific Impact: The SLC enabled precision studies that have contributed to important recent advances in physics. This prototype linear collider also points the way to a larger collider that would enable precision studies of the Higgs boson and other ultraheavy particles thought to have existed in profusion during the Big Bang creation of the universe.

Social Impact: Such facilities help answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. The development and use of such facilities often has practical implications; accelerators have contributed to medical treatments, for example.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.23 World's Most Intense Source of Polarized Electrons



Polarized electron guns at Jefferson Lab.

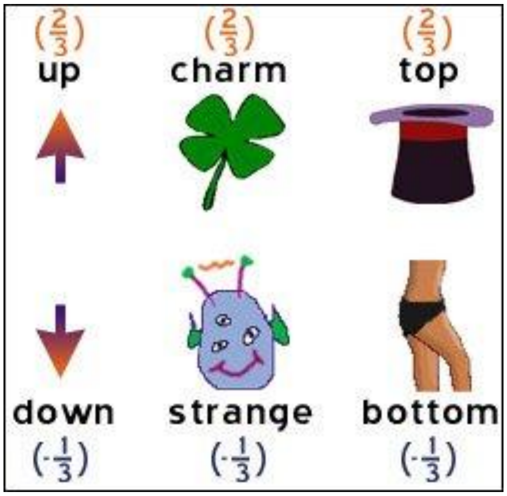
Electron accelerators are widely used to investigate subatomic particles and forces because scientists learn a lot by examining how the electrons' charge and angular momentum (or spin) interact with heavier particles during a collision. Polarized electrons, which act like tiny magnets whose axes are aligned in one fixed direction, produce the cleanest and most informative signals. Recently, Thomas Jefferson National Laboratory developed and installed a very intense and stable source of polarized electrons, the Continuous Electron Beam Accelerator Facility (CEBAF). Using new superconducting radiofrequency (SRF) technology to accelerate the beam, CEBAF produces more polarized electrons in one month than all other electron accelerators have produced in their lifetimes. Unique features of the beam include its precise energy, tiny diameter, high polarization, and continuous time structure (previous electron beams were pulsed). A high-power, continuous beam allows scientists to accumulate data at a high rate, with each interaction sufficiently separated in time to be fully observed. CEBAF is used by more than 1,500 physicists who have submitted more than 300 proposals for use of the unique machine.

Scientific Impact: The facility satisfies a demand for high-current, long-lifetime sources of polarized electrons, which enable scientists to extract otherwise inaccessible information. SRF technology has been adopted for use in several large accelerators abroad and several other Office of Science facilities.

Social Impact: Such facilities help answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. The development and use of such facilities often has practical implications; accelerators have contributed to medical treatments, for example.

SC-Funding Office: Office of High Energy and Nuclear Physics

3.24 Lifetime of the Bottom Quark



The lifetime of a subatomic particle called the "bottom" (or b) quark was first measured at Stanford Linear Accelerator Center in 1983 and found to be unexpectedly long. The measurement provided the value for a missing parameter of the Standard Model, physicists' current theory of matter and the forces of nature. It also led to predictions that the preference of the universe for matter over its mirror image, antimatter, would be seen in decays of the b quark, and made it possible to build "B-factories" to study the matter/antimatter asymmetry. Such studies will help explain why the universe is virtually devoid of antimatter today, even though every particle of matter has a corresponding antiparticle. It is the long b lifetime that produces a finite and measurable separation between the particles produced at B-factories and provides the tool for searching for evidence of the asymmetry. The long lifetime also can be used to separate quark species and for other experimental purposes.

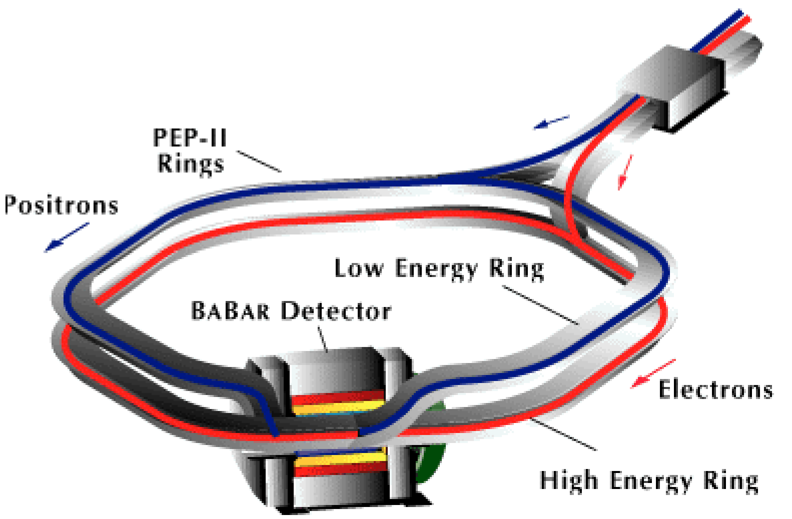
Scientific Impact: This discovery refined scientific knowledge of the parameters that describe the transition strengths among the three known families of quarks. The SLAC work aided in the discovery of the "top" quark (which decays to a b quark) and searches for the Higgs particle, which is the last missing piece of the Standard Model and is expected to decay to pairs of b quarks.

Social Impact: These studies answer questions about the constituents and history of the universe, extending human understanding of nature and contributing to improvements in science education. In addition, although basic research is by definition a search for new knowledge without regard to its practical implications, such work often contributes to technologies with commercial value; examples include computers, lasers, and cancer treatments.

Reference: "Measurement of the Lifetime of Bottom Hadrons," N. S. Lockyer et al., *Phys. Rev. Lett.* 51: 1316 (1983).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.25 New Clues to the Disappearance of Antimatter



Stanford Linear Accelerator Laboratory's Asymmetric B-Factory

All particles of matter have mirror images called antimatter. The universe prefers matter—antimatter is created only in laboratories today—and physicists are not sure why. The answer may lie in differences in the ways unstable particles of matter and antimatter decay, or break down into more stable particles. Physicists now have the accelerators needed to test these differences, thanks to Piermaria Oddone of Lawrence Berkeley National Laboratory, the father of the "B-factory" (so-named because it makes particles containing "bottom" or b quarks). In the late 1980s, Oddone suggested looking for the matter/antimatter asymmetry with a collider of electrons and positrons (anti-electrons) using beams of unequal energy, a radical approach at the time. His proposal led to Stanford Linear Accelerator Laboratory's Asymmetric B-Factory, a collaboration of three national laboratories that began operating in 1999. Researchers use it to measure the decay of B mesons, rare particles that are a mix of matter and antimatter. The asymmetric design allows particles to move in a way that is conducive to study and provides for high luminosity (rate of particle collisions). In 2000, the first results were reported of a breakdown in matter/antimatter symmetry in B mesons.

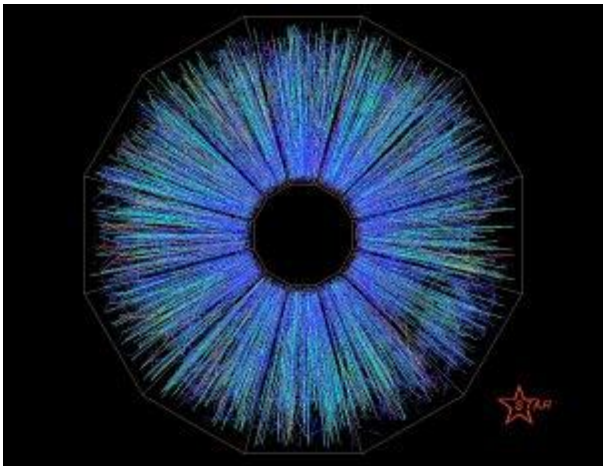
Scientific Impact: The collider design was unprecedented and has achieved luminosities that exceed the previous world record. Operation of the Asymmetric B-Factory promises to provide a stringent test of the Standard Model, physicists' current theory of matter and the forces of nature.

Social Impact: These studies will help humans better understand the origins of the universe and why matter, including the Earth and its inhabitants, exists. (A preference for antimatter in the universe would have annihilated all matter.) In addition, the collider design project produced an electronics technology spin-off, a new methodology for circuit board design and fabrication.

Reference: P. Oddone, *Proceedings of the UCLA Workshop on Linear Collider B B-Factory Conceptual Design*, ed. by D. Stork (1987).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.26 The Highest-Energy Atom Smasher



Thousands of charged particles emerge from a collision of two gold nuclei inside the STAR detector at RHIC.

The highest energies ever recorded in a laboratory were reported in 2000, when Brookhaven National Laboratory began operating its newest "atom smasher," the Relativistic Heavy Ion Collider (RHIC), which collides nuclei at high energies. The first collisions of gold nuclei occurred in June 2000, at energies of 26 trillion electron volts per interaction. Data from this first run imply that conditions will be favorable for creating and studying the quark-gluon plasma—very hot, dense states of nuclear matter that have not existed since microseconds after the Big Bang creation of the universe. The RHIC was made possible by many advances in accelerator technology, instrumentation, and magnets supported by the Office of Science. Images of the event were recorded in stunning three-dimensional detail by the STAR detector, developed in a collaboration of several national laboratories. The RHIC uses as a heavy ion injector the Alternating Gradient Synchrotron, which over four decades has hosted research leading to three Nobel Prizes. New computational methods will enable scientists to model and estimate the properties of subatomic particles and phenomena produced at the RHIC.

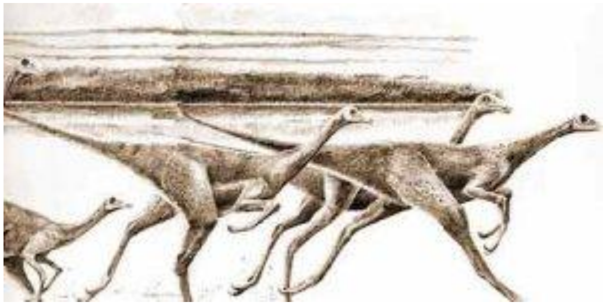
Scientific Impact: Through experiments at the RHIC, scientists will gain insights into the fundamental nature of matter and how has it has evolved since at the dawn of the universe. Development of these machines led to advances in different areas of science, including computer analysis of huge volumes of data and production of superconducting magnets.

Social Impact: Research on fundamental properties of matter typically yields significant technological advances. The RHIC is also a training ground for the next generation of physicists, who may go on to develop new types of computers, medical imaging technologies, cancer treatments, or other ways of observing and controlling the physical world.

Reference: RHIC Design Manual, http://www.rhichome.bnl.gov/NT-share/rhicdm/decades.htm

SC-Funding Office: Office of High Energy and Nuclear Physics

3.27 Why Dinosaurs Are Extinct



In the late 1970s, geologist Walter Alvarez discovered a layer of red clay between fossil-containing limestone deposits in Italy. His father, Nobel laureate Luis Alvarez, suggested how to analyze it. In 1980, neutron activation analysis at Lawrence Berkeley National Laboratory revealed that the clay was rich in iridium, a metal that is scarce in the Earth?s crust but common in extraterrestrial objects. Luis Alvarez then determined the global extent of the iridium, its origin, and the implications. The clay was found at a geological boundary formed 65 million years ago, at a time of mass extinction of many living species, including the dinosaurs. Alvarez suggested that the extinction was initiated by the impact of an asteroid or giant meteor, which caused a dust cloud that blocked much of the sunlight, leading to a drastic and devastating global climate change. This hypothesis, supported by a huge buried crater where a meteorite may have struck the Yucatán Peninsula of Mexico, is considered by many scientists to be the most likely explanation of the dinosaur extinction.

Scientific Impact: This work illustrated the value of the study of isotopes (different forms of the same element) as a tool to better understand the environment; the iridium anomaly has now been identified at more than 75 sites worldwide. This finding also led to development of the controversial Nemesis theory, which postulates that every 26 to 30 million years, a companion star to the sun unleashes a storm of comets, some of which strike the Earth.

Social Impact: The public is fascinated by dinosaurs. This hypothesis answers a long-standing question of great interest to many people, from scientists to schoolchildren.

Reference: "Extraterrestrial cause for the Cretaceous-Tertiary extinction," *Science* (1980).

SC-Funding Office: Office of High Energy and Nuclear Physics

3.28 Understanding and Applying Superstring Theory

Lance Dixon

The Standard Model, physicists' current theory of matter and the forces of nature, is imperfect because it omits gravity and requires 19 input parameters. A possible alternative is superstring theory, which includes gravity and has no input parameters. According to this "theory of everything," all elementary particles and forces and perhaps even the space-time continuum consist of tiny strings under great tension, vibrating and spinning in 10 dimensions. But this theory is very difficult to test or use in calculations. For it to make sense in the real world of four dimensions (space and time), scientists have tried to "hide" the extra six dimensions by curling them up into a space so small that it cannot be probed. Lance Dixon, at Stanford Linear Accelerator Center, and collaborators devised a simpler, easier way to hide the extra dimensions to produce realistic models. With others, he has used superstring theory as a calculation tool for improving theoretical understanding of widely accepted theories. University researchers supported by the Office of Science also have helped establish principles for constructing a superstring model that could contain a realistic unified model of fundamental particles.

Scientific Impact: This work led to an important partnership of high-energy physics and differential geometry research that has generated new insights into the nature of matter and driven new research at the forefront of mathematics.

Social Impact: Eventually, this research could radically change human understanding of the constituents of nature and history of the universe.

Reference: L. J. Dixon et al., *Nucl. Phys.* B294: 43-82 (1987); T. Banks et al., *Nucl. Phys.* B299: 613-626 (1988).

SC-Funding Office: Office of High Energy and Nuclear Physics

4 PLASMA PHYSICS

4.1 Stable Confinement of High-Pressure Plasmas

DIII-D Tokamak at General Atomic

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant energy source in the future. To produce practical amounts of fusion power, plasmas need to be confined at high pressure in a stable condition. Research supported by the Office of Science led to the development and verification of magnetohydrodynamic (MHD) stability theory, which predicts plasma instabilities that limit the stable operating range of devices that confine plasmas using magnetic fields. MHD instabilities can affect magnetic field configurations and cause rapid losses of plasma energy and particles. Using large computer codes, fusion scientists developed MHD stability theory to the point where it can determine plasma stability limits in complex magnetic configurations. Experiments to verify the quantitative predictions spanned two decades because they required the development of new techniques to form and control complex plasma shapes, high-power heating sources to increase plasma pressure, and novel diagnostics for measuring the spatial distributions of plasma pressure and current. Staff at General Atomics, a DOE contractor, received the American Physical Society Award for Excellence in Plasma Physics Research in 1994 for verifying the predicted stability limits of high-pressure plasmas.

Scientific Impact: This work established a solid theoretical foundation for evaluating the stable operating potential of attractive plasma confinement devices, such as tokamaks. Such advances often prove useful in other fields of research that use plasma science and technology, from solar and magnetospheric physics to materials science.

Social Impact: This work will help promote the availability of fusion as an inexhaustible, safe, and environmentally attractive energy source. In addition to the general public, beneficiaries may include industries that use plasma science and technology, including makers of semiconductors and space propulsion systems.

References: “Higher Beta at Higher Elongation in the DIII-D Tokamak," E. A. Lazarus, M. S. Chu, J. R. Ferron, F. J. Helton, *Rev. Mod. Phys.* 59, 175 (1987).

"An Optimization of Beta in the DIII-D Tokamak," E. A. Lazarus, L. L. Lao, T. H. Osborne, T. S. Taylor, *Phys. Fluids* B 4, 3644 (1992).

SC-Funding Office: Office of Fusion Energy Sciences

4.2 The Role of Currents in Plasma Confinement

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant energy source in the future. A key to developing a fusion energy source is the formation and maintenance of the complex magnetic fields that confine the plasma. In a tokamak device, a toroidal current in the plasma is a critical component of the magnetic field. In the 1970s, physicists proposed that the pressure gradient in fusion plasma gives rise to a powerful "bootstrap current." This prediction was confirmed in the 1980s, and the bootstrap current was demonstrated at fusion-relevant temperatures in excess of 100,000,000 °C at Princeton Plasma Physics Laboratory. In addition, with Office of Science support, theorists at the Massachusetts Institute of Technology predicted that radio-frequency electromagnetic waves could produce a net flow of electrons in a tokamak—similar to surfers being moved by a wave—thereby generating a strong current efficiently enough to be useful in a fusion power plant. This research was verified by experiments in Japan and the United States. For this work, researchers from both countries, including scientists from MIT and PPPL, won the American Physical Society Excellence in Plasma Physics Research Award in 1984.

Scientific Impact: This work extended earlier pioneering research on the natural symmetry between thermodynamic forces and the particle fluxes they support, and on wave-particle interactions. It is now possible to maintain and control the magnetic field profile in an advanced tokamak configuration with a combination of bootstrap and radio-frequency wave drive currents.

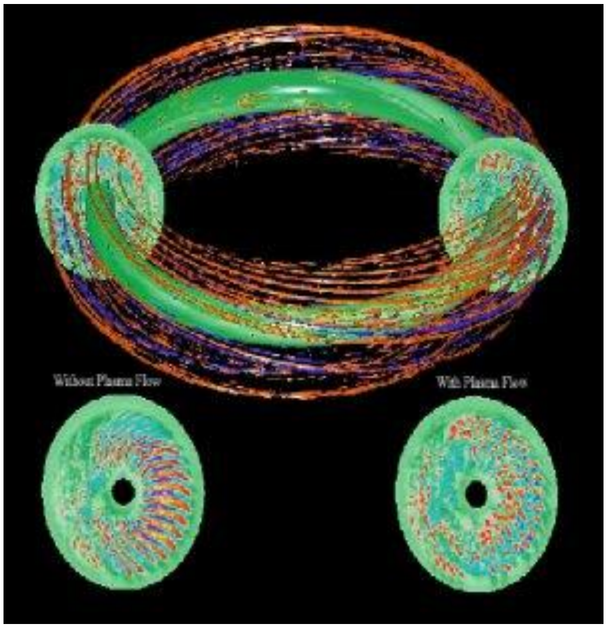
Social Impact: These advances will help promote the availability of fusion as an inexhaustible, safe, and environmentally attractive energy source. In addition to the general public, beneficiaries may include industries that use plasma science and technology, including makers of semiconductors and space propulsion systems.

References: "Theory of Current Drive in Plasmas," Nathaniel J. Fisch, *Rev. Mod. Phys.* 59, 175 (1987).

"Bootstrap Current in TFTR," M. C. Zarnstorff, M. G. Bell, M. Bitter, ..., *Phys. Rev. Lett.* 60, 1306 (1988).

SC-Funding Office: Office of Fusion Energy Sciences

4.3 Reducing Plasma Turbulence



Without plasma flow (left); with plasma flow (right).

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant energy source in the future. Efficient confinement of hot plasma, which is necessary to create fusion energy, is prevented by small-scale instabilities that cause turbulence. Office of Science support has played a major role in efforts to understand and reduce plasma turbulence. U.S. researchers have demonstrated that flow shear (radially varying plasma flow velocities) can suppress the turbulence responsible for transporting particles and energy across the magnetic field in fusion devices. Experimental, theoretical, and computer simulation studies have shown that flow shear produces localized, sharply defined transport barriers that alter the physics of energy and particle transport. The first improved plasma confinement mode resulting from the onset of a sharply defined transport barrier was discovered by German researchers in the early 1980s. More recently, U.S. researchers identified flow shear as the mechanism that produces this edge transport barrier. Sheared flows also have been shown to play a dominant role in the formation of other plasma confinement modes.

Scientific Impact: The enhanced confinement regimes resulting from flow shear stabilization of turbulence are of considerable scientific interest; systems seldom self-organize to a higher energy state, with reduced turbulence and transport, when an additional source of free energy is applied.

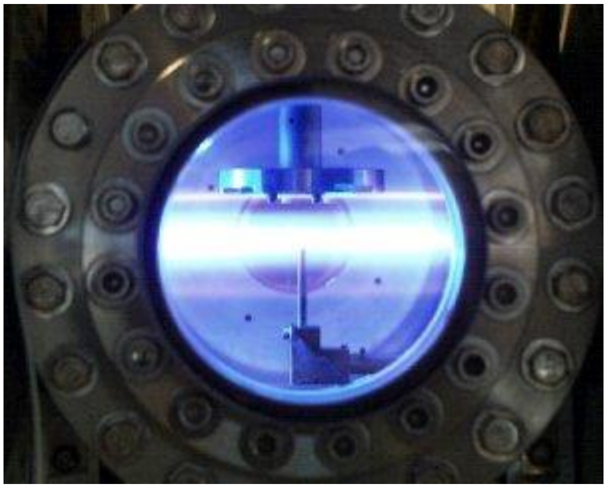
Social Impact: These advances will help promote the availability of fusion as an inexhaustible, safe, and environmentally attractive energy source. In addition to the general public, beneficiaries may include industries that use plasma science and technology, including makers of semiconductors and space propulsion systems.

References: Z. Lin, et al., *Science*, 281, 1835 (1998).

"Comparisons and Physics Basis of Tokamak Transport Models and Turbulence Simulations," A. M. Dimits, G. Bateman, M. A. Beer, B. I. Cohen, et al., Phys. *Plasmas* 7, 969 (2000).

SC-Funding Office: Office of Fusion Energy Sciences

4.4 Measuring the Magnetic Field Inside Plasmas



Helicon Plasma

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant and attractive energy source in the future. An important parameter in plasma science is the current density profile, which is fundamental to the equilibrium, stability, and transport of particles and heat in plasma. Fusion Physics & Technology, Inc., a small business, used DOE funding to develop a technique for measuring the internal magnetic field in fusion plasmas, thus making it possible to determine the current distribution. This technique uses a beam of neutral atoms that propagates across the magnetic field in fusion plasma. The resulting electric field causes a wavelength splitting and linear polarization of the radiation emitted by the beam atoms that are excited by collisions with background gas. The direction of polarization indicates the magnetic field pitch angle, from which scientists can compute the plasma current density profile. This measurement technique was first implemented at the Princeton Plasma Physics Laboratory. The principal investigator, Fred Levinton, received the American Physics Society Award for Excellence in Plasma Physics Research in 1997 for this pioneering work.

Scientific Impact: Results of measurements made with this technique have made important contributions to understanding of the physics of plasmas, especially heat and particle transport, and have provided a basis for comparison with theory. The technique has become widely accepted, and similar instruments are operating on many fusion experiments around the world.

Social Impact: This innovation will help promote the availability of fusion as an inexhaustible, safe, and environmentally attractive energy source. In addition to the general public, beneficiaries may include industries that use plasma science and technology, including makers of semiconductors and space propulsion systems.

Reference: "Magnetic Field Pitch-Angle Measurements in the PBX.M Tokamak Using the Motional Stark Effect," F. M. Levinton, R. J. Fonck, G. M. Gammel, R. Kaita, ..., *Phys. Rev. Lett.* 63, 2060 (1989).

SC-Funding Office: Office of Fusion Energy Sciences

4.5 A New Magnetic Container for Super Hot Plasmas

Spherical torus

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant and attractive energy source in the future. The spherical torus concept creates a unique magnetic field structure to improve plasma stability and confinement at high pressure. This plasma configuration, shaped like a sphere with a narrow hole through the center, can confine a higher plasma pressure for a given magnetic field strength than a conventional tokamak, in which plasma is shaped like a donut. Conceived in 1985 by researchers at Oak Ridge National Laboratory, the spherical torus concept is now being tested at Princeton Plasma Physics Laboratory. Preliminary tests on a small device in the United Kingdom reached a high ratio of plasma pressure to applied magnetic field pressure (called toroidal beta) about 40 percent, that is roughly three times greater than the level reached in a tokamak. Initial results at Princeton are encouraging. The toroidal beta has reached approximately 22.5 percent; and the energy containment efficiency improved by as much as a factor of two when an additional heating method was applied. The goal is to produce and maintain high-performance spherical torus plasmas for pulse lengths of several seconds.

Scientific Impact: Initial results at Princeton suggest that the spherical torus experiment will have adequate heating power to test the theoretically predicted toroidal beta values in the range of 40 percent. This configuration also offers new opportunities to advance the science of high-temperature magnetized plasmas of interest to the astronomical plasma physics community.

Social Impact: Because the amount of fusion power produced is roughly proportional to the square of the plasma pressure, the spherical torus configuration could lead to smaller, less costly development steps to economical fusion power plants. This advance could help promote the availability of fusion as an attractive energy source.

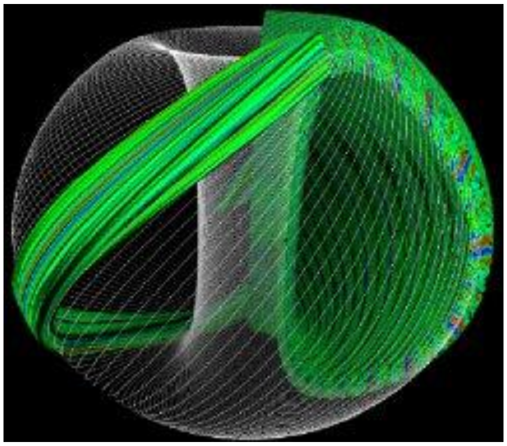
References: "Features of Spherical Torus Plasmas," Y.-K. M. Peng and D. J. Strickler, *Nucl. Fusion* Vol. 26 (1986) 576.

"High-harmonic fast magnetosonic wave coupling, propagation, and heating in a spherical torus plasma," J. Menard, R. Majeski, R. Kaita, M. Ono, T. Munsat, et al., *Phys. Plasmas* 6, 2002 (1999).

"RF Experiments on Spherical torus Plasmas," R. Majeski, J. Menard, D. Batchelor, T. Bigelow, et al., *AIP Conf. Proc.* 485, 296 (1999).

SC-Funding Office: Office of Fusion Energy Sciences

4.6 Modeling Large Systems of Particles



Particle model simulation

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant and attractive energy source in the future. Early pioneers in fusion research developed a powerful method of modeling the behavior of large systems of particles, using the basic equations of motion for interacting charged and neutral particles. The particle-in-cell technique involves dividing the physical space into cells and using statistical methods within individual cells to reduce the number of particles required to model a system. Such simulations have offered insight into the behavior of plasmas in fusion devices by providing predictions of basic spectral and spatial properties of plasma turbulence that can be compared with diagnostic measurements. Researchers with Office of Science funding at University of California campuses in Los Angeles and Berkeley, as well as Stanford University, made important contributions to this work, and an early pioneer won the American Physical Society's James Clerk Maxwell Prize for Plasma Physics in 1977.

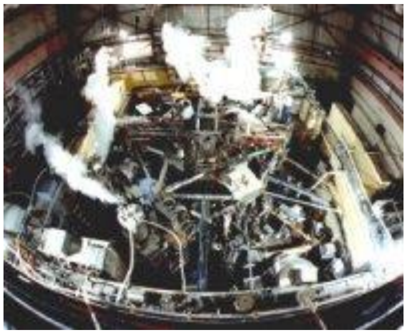
Scientific Impact: This technique has been used to gain many new insights into the behavior of plasmas in confinement devices. The simulations also can be used to validate the analytical treatment of highly nonlinear problems encountered in plasma turbulence such as chaotic and intermittent behavior.

Social Impact: This work contributes to efforts to develop fusion as an attractive energy source. Particle techniques also have been used successfully to study highly nonlinear and turbulent weather patterns, and in smooth particle hydrodynamics to study the dynamics of high-velocity projectiles.

Reference: "Theory of Plasma Simulation Using Finite-Size Particles," A. B. Langton and C. K. Birdsall, *Physics of Fluids* 13, 2115 (1970).

SC-Funding Office: Office of Fusion Energy Sciences

4.7 First Achievement of Fusion Temperatures in the Laboratory



First Achievement of Fusion Temperature in a Laboratory (PLT) Princeton Large Torus

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant and attractive energy source in the future. Scientists at Princeton Plasma Physics Laboratory achieved ion temperatures in excess of 58,000,000 ^{o}C, the minimum required for a self-sustaining fusion reaction (a condition called ignition), for the first time in 1978. These experiments required a number of advances, most importantly in the development of a powerful new technique for heating a magnetically confined plasma-neutral beam heating. The use of neutral beams to heat plasma dates back to the early 1960s with work performed at the Lawrence Livermore and Oak Ridge national laboratories. Neutral beam heating involves the injection of high currents of energetic neutral atoms into the plasma. The neutral atoms cross the magnetic confinement field and enter the plasma, where they are ionized and confined by the magnetic field. They then heat the plasma through collisions with the plasma ions and electrons. Oak Ridge supplied the neutral beam heating systems used in the Princeton experiments.

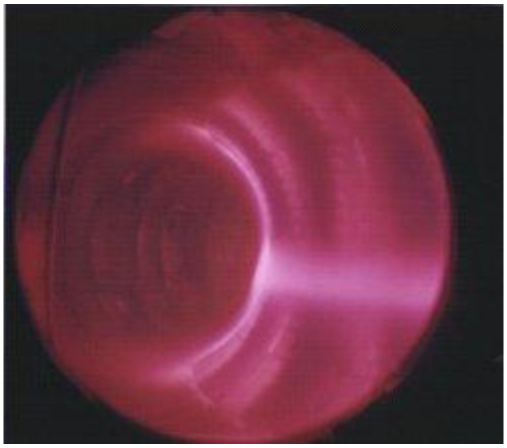
Scientific Impact: Neutral beam heating paved the way for major advances in the next generation of plasma confinement devices, which attained ion temperatures suitable for practical fusion energy production and multi-megawatt fusion power levels. It is believed that practical fusion power production will require plasma temperatures in the range of 100,000,000 ^{o}C to 200,000,000 ^{o}C.

Social Impact: This advance helped lay the groundwork for promoting fusion as an attractive energy source. In addition to the general public, beneficiaries may include industries that use plasma science and technology, including makers of semiconductors and space propulsion systems.

Reference: "Neutral-beam-heating results from the Princeton Large Torus," H. Eubank, R. Goldston, V. Arunasalam, M. Bitter, ..., *Phys. Rev. Lett.* 43, 270 (1979).

SC-Funding Office: Office of Fusion Energy Sciences

4.8 A New Plasma Confinement Regime



TFTR Plasma Discharge

Plasma science (the study of ionized gases) is critical to the development of fusion energy (involving the fusion of nuclei), which could be an abundant and attractive energy source in the future. Scientists at the Princeton Plasma Physics Laboratory recently discovered a new plasma confinement regime. By decreasing the influx of neutral gas from the walls of the vacuum chamber containing the plasma, they obtained peak plasma density profiles and high ion temperatures. This led to a reduction in energy loss by a factor of two to three and an increase in the number of thermonuclear fusion reactions by a factor of about 20. Scientists later used this enhanced confinement regime to produce 10.7 million watts of fusion power, with a total yield of 4.2 million joules, in a deuterium-tritium plasma. (A deuterium-tritium fusion reaction produces a neutron and an alpha particle [helium-4 nucleus], while mass is converted to energy. The neutron carries away 80 percent of this energy, and the rest goes to the alpha particle. In a fusion power plant, the neutron energy would be converted to heat to make steam for the generation of electricity; the alpha particle energy is transferred to the plasma and, when sufficient to sustain the plasma temperature, the plasma is "ignited.") Three scientists won the American Physical Society Award for Excellence in Plasma Physics Research in 1988.

Scientific Impact: The enhanced confinement regime was used to study the confinement of fusion-produced alpha particles. The scientists determined that alpha particle confinement and loss agreed with theoretical predictions, and they observed the first indications of alpha particle heating of the background plasma.

Social Impact: This advance helped lay the groundwork for promoting fusion as an attractive energy source. If converted to electricity, the 10.7 million watts of fusion power produced in this experiment would meet the needs of about 3,000 average-sized homes.

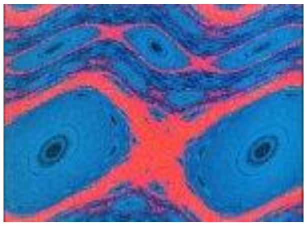
References: "High Temperature Plasmas in a Tokamak Fusion Test Reactor," J. D. Strachan, M. Bitter, A. T. Ramsey, ..., *Phys. Rev. Lett.* 58, 1004 (1987).

"Fusion Plasma Experiments on TFTR: A 20-year Retrospective," R. J. Hawryluk, S. Batha, W. Blanchard, M. Beer, ..., *Phys. Plasmas* 5, 1577 (1998).

SC-Funding Office: Office of Fusion Energy Sciences

5 ADVANCED SCIENTIFIC COMPUTING RESEARCH

5.1 Emergence of Chaotic Systems



Kolmogorov Arnold Moser Map

Sir Isaac Newton (best known for proposing the law of gravity in 1687) suggested a deterministic set of laws implying that the future is determined fully by the present. But since the mid-1970s, scientists have come to agree that determinism is transitory and may give way to chaotic behavior. Research at Los Alamos National Laboratory and a number of universities led to an understanding of the emergence of chaotic behavior in systems thought to be deterministic, a concept that has gained widespread acceptance in almost every discipline of science and mathematics. Early studies of nonlinear maps at Los Alamos led to the discovery of universality in the transition to chaos, described in the lab's most highly cited paper to date. This concept provides a fundamental understanding of the relationship between microscopic behavior of classical systems and macroscopic behavior dominated by statistical properties. Chaotic systems appear in many natural or engineered contexts. Strategies for control of such systems have been developed, with important implications for chemical engineering and fluid flow.

Scientific Impact: The concepts of chaos have changed how scientists view the dynamics in physical systems. In the early 1980s, few scientists believed in deterministic chaos; today, virtually all branches of science and engineering interpret nonrandom dynamics in the language of chaos, and all accept that chaos is an important advance in understanding of such systems.

Social Impact: These ideas have been implemented successfully in predicting nonlinear time series in financial markets, forecasting short-term weather, diagnosing and controlling medical conditions such as heart fibrillation, understanding stability in engineering structures and devices, and designing chaotic encryption schemes. Chaos theory also has changed, to some degree, the way the general public perceives science.

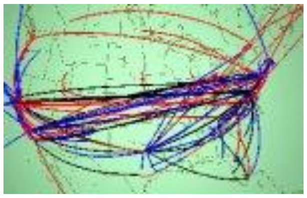
References: Feudel, U; Grebogi, C., "Multistability and the control of complexity," *Chaos* (Woodbury, N.Y.) Dec 31, 1997, ISSN 1054-1500.

Barreto, E; Hunt, B.R; Grebogi, C; Yorke, J.A., "From High Dimensional Chaos to Stable Periodic Orbits: The Structure of Parameter Space," *Physical Review Letters*, Jun 30, 1997, ISSN 0031-9007.

Auerbach, D.; Grebogi, C.; Ott, E.; Yorke, J.A., "Controlling chaos in high dimensional systems," *Physical Review Letters*, Dec 14, 1992, ISSN 0031-9007. Feigenbaum, M.J., "Quantitative universality for a class of nonlinear transformations," *J. Stat. Phys.*, Jul 31, 1978.

SC-Funding Office: Office of Advanced Scientific Computing Research

5.2 The Launch of Internet Conferencing



Internet Videoconferencing Backbone in US MBONE

From round-the-clock coverage of space shuttle flights to international broadcast of a complex liver operation to a Rolling Stones concert, the use and influence of the Internet has been extended by the multicast backbone (M-Bone). First used in a broadcast in 1992, M-bone is a virtual network that sends compressed audio/video data packets to multiple remote locations on the Internet as one data stream, minimizing duplicate transmissions. M-Bone enables users worldwide to not only see and talk to one another, but to also work on a shared electronic window called a whiteboard, or "infinite piece of paper." A principal creator was Van Jacobson of Lawrence Berkeley National Laboratory, whose team developed most of the user-friendly software tools. Although simple in concept, M-Bone is unique in its capability to dynamically construct distribution trees using the shortest, most efficient paths. This high level of efficiency is necessary to prevent congestion and collapse of the Internet, because the broadcasts usually include live video, which generates large volumes of data.

Scientific Impact: M-bone launched a new era in scientific collaboration. Not long after its introduction, M-bone was put into service routinely for collaborative work by more than 10,000 users at federal agencies and other sites in 30 countries.

Social Impact: More democratic than traditional videoteleconferencing, which joins a few sites with expensive dedicated transmission lines. M-Bone links anyone who has a workstation with audiovisual capabilities and a high-speed connection to the Internet.

Reference: Deering, S., Estrin, D., Farinacci, D., Jacobson, V., Lui, C., and Wei, L., "The PIM Architecture for Wide-Area Multicast Routing," *IEEE/ACM.*

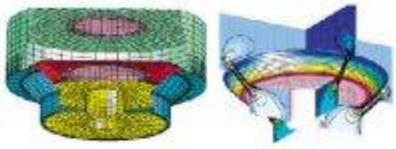
Transactions on Networking, Vol.4, No.2, April 1996. An earlier version, "An Architecture for Wide-Area Multicast Routing," appeared in *SIGCOMM 1994*, August 1994, pp. 126-135.

McCanne, S., and Jacobson, V., vic: "A Flexible Framework Framework for Packet Video," *ACM Multimedia '95*, November 1995, San Francisco, CA, pp. 511-522. (Best student paper award.)

Schulzrinne, H., Casner, S., Frederick, R., and Jacobson, V., "RTP: A Transport Protocol for Real-Time Applications," *RFC* 1889, January 1996.

SC-Funding Office: Office of Advanced Scientific Computing Research

5.3 Fluid Dynamics Calculations in Complex Geometries



Flow past a diesel engine valve.

In the 1990s, scientists from several national laboratories developed a framework for simulating fluid flow in a complex, moving geometry using a method of overlapping grids. Known as Overture, this work demonstrated that carefully engineered software frameworks improve the efficiency and ease of development of large parallel software systems used to study important physical systems such as combustion. Because of its object-oriented design, Overture reduces code duplication, encourages interoperability of application software, and simplifies the learning curve for new computational methods. The architecture provides flexibility to address a wide range of applications that involve simulations in complex moving geometry on serial and parallel computers. Advantages include broader, more in-depth research into numerical methods for scientific and industrial applications. Lawrence Berkeley, Lawrence Livermore, and Los Alamos national laboratories participated, along with the Courant Institute.

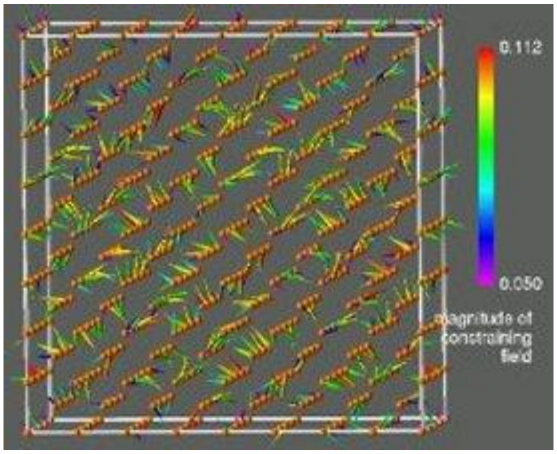
Scientific Impact: Overture, available on the World Wide Web as an open source, has greatly simplified the development of scientific simulations in complex geometries. It has enabled worldwide research collaborations in a variety of areas, from simulation of the combustion of reactive fluids for diesel engine simulation to studies of the mechanisms for nutrient uptake by plant roots.

Social Impact: The software approach developed here forms the basis for calculations of fluid flow with important implications for diesel engine design and other combustion problems, aerodynamics, and chemical processing. These processes are important elements of the Nation's energy supply.

Reference: D. L Brown and W. D. Henshaw, "OVERTURE: Object-oriented tools for solving CFD and combustion problems," in *High Performance Computing 1998, Grand Challenges in computer Simulation*, A. Tentner, ed., pages 21-26, The Soc. for Computer Simul. Int'l, 1998.

SC-Funding Office: Office of Advanced Scientific Computing Research

5.4 Best Performances in Scientific Computing



A computer code written recently to simulate how materials behave on the microscale has had a macroscale impact on scientific computing. Researchers from Oak Ridge National Laboratory, the National Energy Research Supercomputing Center, and colleagues wrote the code in 1998 to simulate the behavior of iron atoms and thereby provide a better microscopic understanding of metallic magnetism. Using a new "spin dynamics" technique developed at Ames Laboratory, the team wrote a computer program that executed the equations of motion for as many as 1,024 atoms. When this work was performed using special supercomputers, the running code was able to sustain a record-setting speed that surpassed one thousand billion operations per second (or 1 teraflop). This work won the 1998 Gordon Bell Award for the best performance of a real application code, and was the 2000 Computerworld Smithsonian Laureate for the first teraflop-scale application code. This remains the fastest sustained real application ever run on supercomputers.

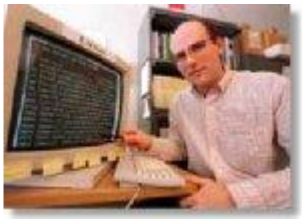
Scientific Impact: This calculation demonstrated that terascale computing could lead to new science and provided new insight into the behavior of magnetic materials. High-performance computing has become a crucial tool for scientific discovery in many fields, including materials research, climate prediction, and bioinformatics.

Social Impact: Understanding of metallic magnetism is key to many technologies, including magnetic data storage devices and motors. This work has important implications for future research in high-performance computer disk drives and magnetic recording media, as well as power generation and use.

Reference: Balazs Ujfalussy, Xindong Wang, Xiaoguang Zhang, D. M. C. Nicholson, W. A. Shelton and G. M. Stocks, Oak Ridge National Laboratory; A. Canning, NERSC, Lawrence Berkeley National Laboratory; Yang Wang, Pittsburgh Supercomputing Center; B. L. Gyorffy, H. H. Wills Physics Laboratory, UK. "High Performance First Principles Method for Non-Equilibrium States in Magnets," in *Proceedings of SC98 Conference*, November 7-13, 1998, Orlando, Florida, sponsored by IEEE Computer Society and ACM SIGARCH.

SC-Funding Office: Office of Advanced Scientific Computing Research and Office of Basic Energy Science

5.5 Mathematics Puzzle Finally Solved



Dr. William McCune at Argonne Labs, Illinois in his office with computer. The "Proof of Robbins Conjecture" problem is on the screen. Photo credit: Lloyd DeGrane/*The New York Times*

In the early 1930s, Herbert Robbins of Harvard University posed a question that intrigued mathematicians: Is a particular set of three equations powerful enough to capture all the laws of Boolean algebra? (Boolean algebra is a mathematical model of basic rules of logic and thought; it obeys laws such as: "For any proposition P, the negation of the negation of P means the same thing as P"). Some of the great mathematicians of the century worked on the problem, but the solution was not forthcoming until 1996, when Argonne National Laboratory used powerful automated reasoning software to conclude that yes, one set of rules can capture all the laws of Boolean algebra. Key to the 15-step proof was a system called EQP (equational prover) and a new strategy, both written by William McCune. The problem was so difficult that solving it required more that eight days of computer time on a number of Unix workstations.

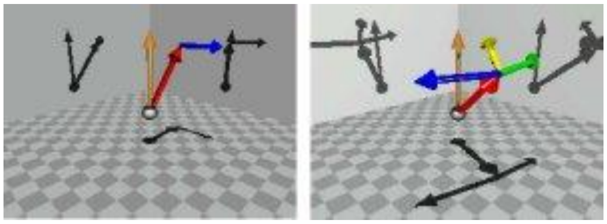
Scientific Impact: This work, cited as a major accomplishment in artificial intelligence, demonstrated that automated reasoning programs can be used as powerful reasoning assistants. Unlike previous attempts to prove famous theorems using special-purpose software, this work relied on a general-purpose program, which produced a relatively short proof that can be verified by hand or by independent proof-checking programs.

Social Impact: This problem was solved using spare computer time at smaller computers around the world, suggesting that many other complex problems can be addressed without expensive supercomputers. Furthermore, the mathematicians collaborated without regard to institutional or even international borders, and without a research grant.

Reference: "Solution of the Robbins Problem," W. McCune, *Journal of Automated Reasoning* (JAR) 19(3), 263-276 (1997).

SC-Funding Office: Office of Advanced Scientific Computing Research

5.6 Accurate Modeling of Magnetic Materials



Modeling of spins at zero and finite temperatures.

Not long ago, techniques for modeling and evaluating magnetic materials were too simplistic to reproduce accurately all the data obtained in experiments. But in 1995, researchers at Ames Laboratory, led by Bruce Harmon, developed a "spin dynamics" computational technique that can be used to accurately represent and evaluate the fluctuations of atomic moments (magnetic orientations) in solid magnetic materials at different temperatures. Among its benefits, the method can be used to make calculations of realistic-sized systems at temperatures of practical and scientific interest. Using this technique, scientists for the first time theoretically determined the magnetic moments in iron and nickel at high temperatures, even above a key temperature at which the magnetic moments vary in magnitude and point in random directions. Current studies focus on how and why specific defects in permanent magnets are crucial in determining desirable magnetic properties. Oak Ridge National Laboratory and collaborators used the technique in a record-setting supercomputer calculation.

Scientific Impact: The spin dynamics approach is a significant contribution to the foundations of a new theory of the dynamics of magnetic moments at finite temperature and in response to external applied fields. It enables scientists to model material properties at room temperature, at which magnets typically are used.

Social Impact: Metallic magnetism is key to many technologies, including magnetic data storage and electric power generation devices. Accurate modeling of computer bit switching is essential for the design of future high-density computer disks, and the capability to optimize high-temperature magnetic materials will lead to more energy efficient motors and transformers.

Reference: *Phys. Rev. Lett.*, 75,729 (1995).

SC-Funding Office: Office of Advanced Scientific Computing Research

5.7 The Transition to Massively Parallel Supercomputing

Transition to parallel computing computers from left to right: Cray x-MP, Cray 2, Cray c-90, Paragon, CM-5, Cray T3-E, Nirvana Blue, ASCI Red, IBM SP

Supercomputers are plenty fast, but a number of them working in parallel are orders of magnitude faster. Researchers at several national laboratories and universities supported by the Office of Science produced the software, scalable operating systems, and other technologies needed for massively parallel supercomputing (involving 1,000 or more processors) and demonstrated its value in fields ranging from seismic imaging to materials modeling. In one example, Oak Ridge National Laboratory and collaborators developed Parallel Virtual Machine (PVM) software, which allows heterogeneous collections of computers—even personal computers and workstations—to be linked together regardless of location, and treated as one parallel computer. This software, first released publicly in 1991, led to the development of cluster computing, in which many inexpensive machines are connected to create a powerful system. Argonne National Laboratory developed software that provides a portable environment for building, running, and examining the performance of programs in a wide variety of parallel computing environments. The combined work on massively parallel systems has won three Gordon Bell awards and six R&D 100 awards from *R&D Magazine* recognizing significant new technologies, and received numerous patents.

Scientific Impact: Massively parallel computing can solve problems up to 100 times faster than serial supercomputers. PVM has tens of thousands of users in scientific and other fields and has become the de facto global standard for distributed computing; thousands of programmers use the Argonne software, which increases productivity by enabling applications development on diverse architectures without program performance losses or time-consuming code changes.

Social Impact: The growing popularity of parallel computing for industrial and medical applications is exemplified by wide use of PVM, which helps many large companies design new products cost effectively. PVM also is used as an educational tool, enabling universities without access to parallel computers to teach parallel programming courses.

Reference: van der Weide, E.; Deconinck, H.; Issman, E.; Degrez, G., "A parallel, implicit, multi-dimensional upwind, residual distribution method for the Navier-Stokes equations on unstructured grids," *Computational Mechanics*, Mar 25, 1999, ISSN 0178-7675.

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ScaLAPACK Users' Guide, L.S. Blackford, J. Choi, A Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, R.C. Whaley, SIAM, Philadelphia (1997).

SC-Funding Office: Office of Advanced Scientific Computing Research

5.8 Identifying an Intractable Scientific Problem

Sandia researcher Sorin Istrail and the Ising model, developed by Ernst Ising in 1926 as part of his PhD dissertation.

Some scientific problems simply cannot be solved. One such problem was identified in 2000 by computational biologist Sorin Istrail at Sandia National Laboratories, who proved that the solution of the much-studied Ising model cannot be extended to three dimensions (3D). The original model, developed by Ernst Ising in 1926 as part of his Ph.D. dissertation, often is used to describe wide-ranging changes in state, from flocking birds to unison freezing of water molecules. Ising conceived of the model in one dimension; later, Nobel laureate Lars Onsager extended it to two dimensions. But the world's top mathematical physicists failed to provide the exact solution for the 3D Ising model; its properties can be determined numerically with high accuracy, but not exactly, not for any lattice, and not in terms of elementary equations. Istrail explained why, using a method called computational intractability, which identifies problems that cannot be solved in humanly feasible time. Approximately 6,000 such problems are known among all areas of science.

Scientific Impact: The work eliminated scientific uncertainty about the exactness of the 3D Ising model, thus ensuring that scientists would not waste time trying to solve the unsolvable. Fundamental problems in physics hinge on whether such models are fully understood.

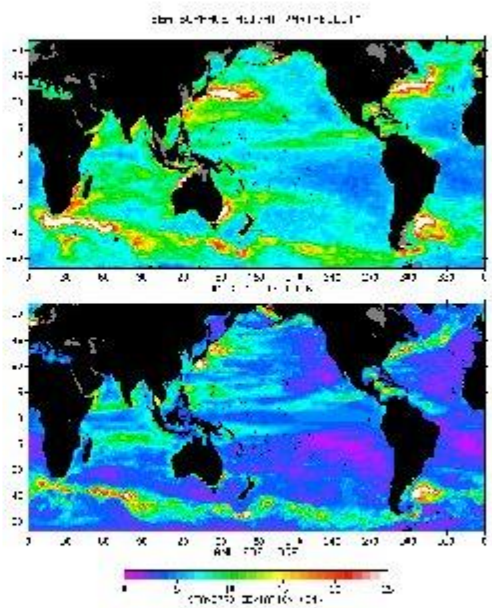
Social Impact: Because most real-world problems occur in 3D, this work effectively eliminated the possibility that the Ising Model will ever have a direct social impact. But indirectly, this work has saved money by encouraging the direction of scientific efforts toward other, more fruitful areas.

Reference: "Statistical Mechanics, Three-Dimensionality and NP-completeness: Universality of Intractability for the Partition Function of the Ising Model Across Non-Planar Lattices," *Proceedings of the 31st ACM Annual Symposium on the Theory of Computing* (STOC 2000), May 21-23, 2000, Portland, Oregon. ACM Press 2000.

SC-Funding Office: Office of Advanced Scientific Computing Research

6 BIOLOGICAL AND ENVIRONMENTAL RESEARCH

6.1 Improving the Realism of Global Simulations



Sea surface height variability: satellite measurements (top) vs model predictions (bottom). (Click here to see larger version.)

Computer simulations of the Earth's climate are more accurate than ever now, thanks to recent advances in ocean modeling using massively parallel computers. With their expertise in fluid dynamics modeling and associated numerical methods, Los Alamos National Laboratory scientists restructured an old ocean circulation model and introduced new algorithms for key processes and boundary conditions to build the Parallel Ocean Program (POP). The model has sufficient spatial resolution (0.1 degree latitude and longitude, compared to the previous 0.5 degree state of the art) and new formulations for transport and diffusion needed to simulate energy-containing eddies. With POP, researchers carried out the first dynamical simulations of global ocean circulation that explicitly and correctly simulated the transport of heat by ocean currents. The simulation then was compared with observations, a key step in the development of realistic models for regional climate studies. Both POP and Los Alamos' innovative approach to modeling sea ice dynamics (called CICE) have been incorporated into the latest climate system model used by the National Center for Atmospheric Research.

Scientific Impact: The enhanced resolution provides a new level of realism for global simulations; many important aspects of Atlantic Ocean circulation have been captured accurately for the first time. Both POP and CICE have growing user communities, including oceanographers.

Social Impact: Explicit simulation of ocean heat transport will enable scientists to model and predict climate variations and long-term climate change. The models could be used to simulate projected climate change under different anthropogenic emission scenarios, and thus contribute to sound policy making and a better quality of life for future generations.

Reference: L.-L. Fu and R. D. Smith, "1996: Global ocean circulation from satellite altimetry and high-resolution computer simulation," *Bull. Am. Meteor. Soc.*, 11:2625-2636.

M. E. Maltrud, R. D. Smith, A. J. Semtner, R. C. Malone, "1998: Global eddy resolving ocean simulations driven by 1985-1995 atmospheric winds," *J. Geophys. Res.*, 103:30825-30853.

R. D. Smith, M. E. Maltrud, F. O. Bryan, and M. W. Hecht, "2001: Numerical Simulation of the North Atlantic Ocean at 1/10º," *J. Phys. Oceanogr.*, 30:1532-1561.

SC-Funding Office: Office of Biological and Environmental Research

6.2 Decoding the Human Genome

Scientists are close to completing the genetic blueprint for a human being, thanks in large part to Office of Science funding. DOE was the first federal agency to propose that the human genome could be sequenced, and it launched the Human Genome Project in 1986. Today, DOE's Joint Genome Institute (a consortium of three laboratories) is one of the 16 institutions that constitute the Human Genome Sequencing Consortium, which recently announced completion of a working draft of the human genome. About one-fourth of the chemical sequence was finished and another half was in near-finished form or better. Contributing to that achievement was the JGI's completion of high-quality draft sequences of chromosomes 5, 16, and 19, which together contain some 12,000 genes, including those implicated in forms of kidney disease, prostate and colorectal cancer, leukemia, hypertension, diabetes, and atherosclerosis. The JGI's DNA Production Genomics Facility is one of the most productive and cost-effective public-sector DNA sequencing laboratories in the world.

Scientific Impact: The large-scale sequencing work will provide a framework for efficiently answering many questions in biology, such as the number of human genes, recently estimated to be much lower (30,000) than previously thought (100,000). The JGI aims to develop and use new sequencing and computational technologies with the goal of discovering and characterizing the basic principles and relationships underlying living systems.

Social Impact: Armed with the DNA sequence of the human genome, scientists will be able to identify more genes responsible for countless diseases and develop diagnostic and treatment approaches. Genomic studies also should answer profound questions, such as why some people are able to defend themselves against the AIDS virus and others are not.

Reference: "Initial sequencing and analysis of the human genome. The Genome International Sequencing Consortium." *Nature* 409, 860-921 (15 February 2001).

SC-Funding Office: Office of Biological and Environmental Research

6.3 Verifying the "Third Branch of Life"

Electron micrograph and genetic map of *Methanococcus jannaschii*

Archaea look like bacteria, but biochemically and genetically, they are quite different. For example, archaea can thrive in extreme conditions that would kill other life forms. In the late 1970s, these unusual organisms were first recognized as distinct from eukaryotes (plants, animals, and other organisms whose cells have a nucleus) and prokaryotes (or bacteria, whose cells contain no distinct nucleus). This finding was verified in 1996, when a study funded by the Office of Science's Microbial Genome Initiative mapped the entire genome sequence of *Methanococcus jannaschii* and thereby confirmed its place in the "third branch of life," separate from prokaryotes and eukaryotes and ancestral to both. About two-thirds of the genes of *M. jannaschii*, a microbe from boiling vents deep in the Pacific Ocean, looked like nothing seen before in biology. The genes involved in energy production, cell division, and metabolism were similar to those in bacteria, whereas those involved in DNA transcription, translation, and replication were similar to those found in eukaryotes.

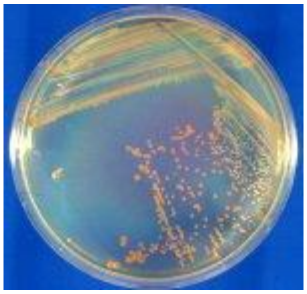
Scientific Impact: This work confirmed that archaea are separate and distinct life forms and provided the information needed to compare the three domains of life at the genomic level. M. jannaschii is also worthy of study in itself; it produces methane as a by-product of metabolism, thus offering the possibility of generating large supplies of a safe and renewable source of energy.

Social Impact: This microbe makes hundreds of enzymes that are stable at high temperatures and therefore could have practical uses in medicine, food science, and other industries. This type of research helps DOE understand the effects and by-products of energy production and identify organisms useful in environmental cleanup.

Reference: Bult, C.J., White, O., Olsen, G.J., Zhou, L., Fleischmann, R.D., Sutton, G.G., Blake, J.A., FitzGerald, L.M., Clayton, R.A., Gocayne, J.D., Kerlavage, A.R., Dougherty, B.A.,Tomb, J.F., Adams MD, Reich CI, Overbeek R, Kirkness EF, Weinstock KG, Merrick JM, Glodek, A., Scott, J.L., Geoghagen, N.S., Venter, J.C., "Complete genome sequence of the methanogenic archaeon, Methanococcus jannaschii," *Science* 273:1058-73 (1996).

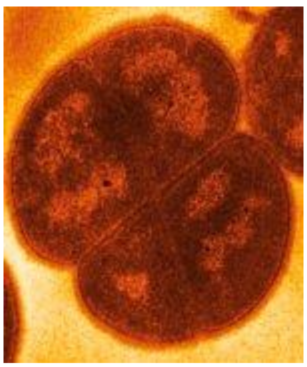
SC-Funding Office: Office of Biological and Environmental Research

6.4 The World's Toughest Microbe



Electron micrograph of a four-cell cluster of Deinococcus radiodurans.

A bacterium first discovered in spoiled beef and believed sterilized by radiation turned out to be "Conan the Bacterium" (aka Superbug)—the most radiation-resistant life form ever found. *Deinococcus radiodurans* is highly resistant to genotoxic chemicals, oxidative damage, high levels of ionizing and ultraviolet radiation, and desiccation; it can survive 3,000 times the radiation dose that is lethal to humans. The capability to survive in such extreme environments is attributed in part to a unique DNA repair system in combination with its chromosome copy number and structure. Researchers supported by the Office of Science reengineered the microbe so that it can reduce toxic metals and partially degrade harmful solvents while surviving the high radiations levels typical of those at DOE waste sites. This was the first time a microbe has been engineered to have these remarkable capabilities. The DNA of this organism was sequenced with Office of Science support as well.



Scientific Impact: This work established both the capability to engineer additional functions into *D. radiodurans* and the persistence of the added functionality despite exposure to radiation. Studies of this microbe will add to understanding of sensitive enzymes responsible for monitoring and repairing damage to DNA caused by radiation and other agents.

Social Impact: The astonishing DNA repair capacities of this organism, as well as the feasibility of genetically modifying it, are of interest for cleanup of radioactive wastes. The techniques used to modify the microbe could lead to new biological solutions—rather than traditional, costly "pump and treat" options—for cleaning up environmental contamination resulting from the production of weapons-grade nuclear materials in years past.

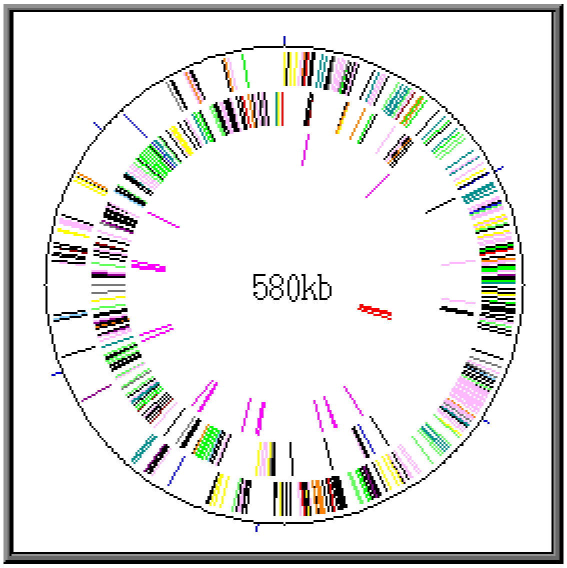
Deinococcus radiodurans growing on agar plates in the presence of 6000 rads per hour of radiation.

Reference: K. S. Makarova, L. Aravind, L.Tatusov, Y. I. Wolf, E. V. Koonin, and M. J. Daly, "Genome of the extremely radiation resistant bacterium Deinococcus radiodurans viewed from the perspective of comparative genomics," *Microbiology and Molecular Biology Reviews*, 65, 44-79 (2001).

H. Brim, S. McFarlan, L. Wackett, K. W. Minton, M. Zhai, J. Fredrickson, and M. J. Daly, "Engineering Deinococcus radiodurans for metal remediation in radioactive mixed waste environments," *Nature Biotechnology*, 18, 85-90 (2000).

SC-Funding Office: Office of Biological and Environmental Research

6.5 The Smallest Genome that Sustains Independent Life



Genetic map of Mycoplasma genitalium

Humble microbes are assuming great importance in genetic studies, thanks to the Office of Science's Microbial Genome Program, launched in 1994. The program goal is to sequence microorganisms of interest to DOE's energy and environmental cleanup programs. The first genome completed was that of *Mycoplasma genitalium*, a tiny pathogen. When the entire 580,000-unit DNA sequence was completed, this free-living microbe was discovered to have only 470 genes that code for proteins. The human genome, by comparison, recently was estimated to contain some 30,000 genes (less than one-third of previous estimates but still a relatively large number). The tiny genome of *M. genitalium* is the smallest known for a self-replicating, free-living organism, although even smaller ones may exist. Mycoplasmas are parasites for a wide range of hosts, including humans, animals, insects, and plants.

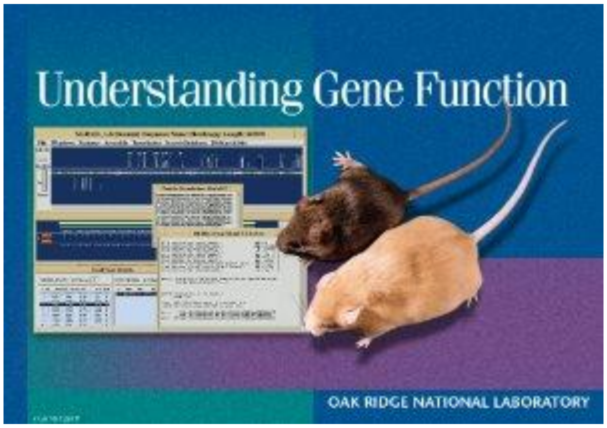
Scientific Impact: : *M. genitalium* provides researchers with a model for the minimum number of genes and protein products necessary for independent (host-free) existence. Microbial genomics, now one of the hottest fields in science, may reverse the traditional paradigm of biology, which until recently has relied on deductions about a single organism's genetic controls from observations of behavior and inheritance.

Social Impact: Knowing the minimum complement of genes an organism needs to be free-living is an essential step toward engineering microbes for a wide range of practical uses. These uses could support DOE missions such as energy production and environmental cleanup.

Reference: "The minimal gene complement of Mycoplasma genitalium," Fraser, C.M., Gocayne, J.D., White, O., Adams, M.D., Clayton, R.A., Fleischmann, R.D., Bult, C.J., Kerlavage, A.R., Sutton, G., Kelley, J.M., et al., *Science* 270:397-403 (1995).

SC-Funding Office: Office of Biological and Environmental Research

6.6 Speeding Up the Process of Gene Discovery



GRAIL will increasingly provide clues about gene regulation by generating comparative information for closely related genomes such as human and mouse.

The human genome contains information that could be used to prevent birth defects and treat or cure devastating diseases, but it is written in a language that scientists are only beginning to understand. To help decipher the code, Ed Uberbacher and colleagues at Oak Ridge National Laboratory combined cutting-edge computer technology with their knowledge of human biology to develop GRAIL (for Gene Recognition Analysis Internet Link), a "thinking" computer program that imitates the human learning process as it searches for genetic meaning. GRAIL and successor software programs can rapidly identify key instructions in genes from within vast stretches of DNA that appear to be meaningless—a critical contribution to the massive, international effort to record and understand the billions of bits and pieces of DNA that make up the human genome, which contains an estimated 30,000 genes. Like humans, GRAIL learns by observing. To train the program, the scientists developed seven statistical rules differentiating genes from other parts of DNA. As it examines more and more bits of DNA, the program learns when and how well the rules work and adjusts them accordingly.

Scientific Impact: About 1,000 biotechnology companies and laboratories now use GRAIL to track down genes that play a role in human disease. The program has become increasingly productive over time and greatly accelerated the process of locating human genes.

Social Impact: In a recent application, GRAIL located the gene that causes adrenoleukodystrophy, an often-fatal disease of the nervous system that affects young boys. Identification and understanding of such genes could lead to treatments or cures for conditions ranging from sickle-cell anemia to muscular dystrophy and cystic fibrosis.

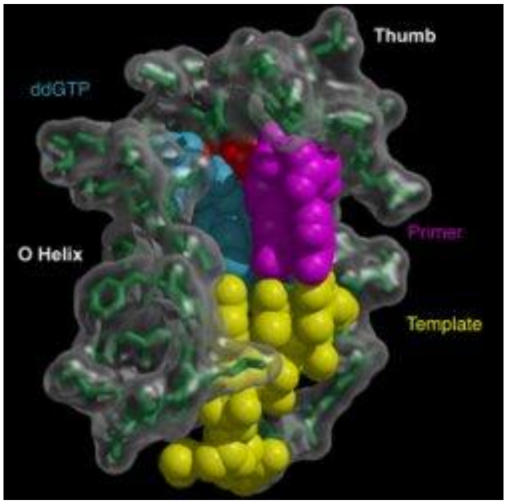
Reference: E.C. Uberbacher and R.J. Mural, "Locating Protein Coding Regions in Human DNA Sequences Using a Multiple Sensor-Neural Network Approach," *Proc. Natl. Acad. Sci.* USA, Vol. 88, pp. 11261-11265 (1991).

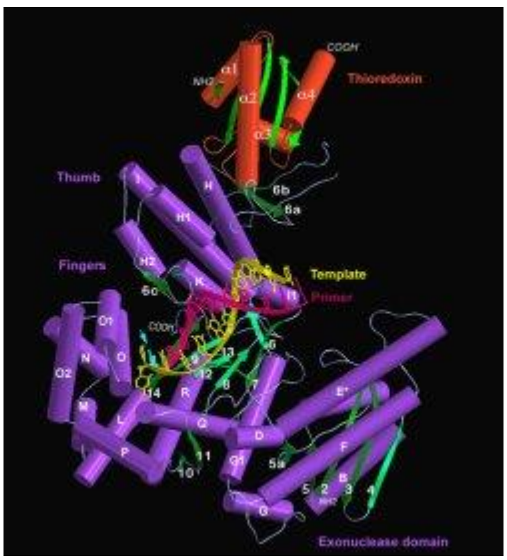
Edward C. Uberbacher, Ying Xu, and Richard J. Mural, "Discovering and Understanding Genes in Human DNA Sequence Using GRAIL," *Comput. Methods Macromol. Sequence Anal.*, Vol. 266, pp. 259-281, 1996.

Ying Xu and Edward C. Uberbacher, "Automated Gene Identification in Large-Scale Genomic Sequences," *Journal of Computational Biology*, Vol. 4.3, pp. 325-338, 1997.

SC-Funding Office: Office of Biological and Environmental Research

6.7 Engineered Enzyme Accelerates DNA Sequencing





Models of the structure of T7 DNA polymerase bound to a DNA substrate molecule.

The international effort to decode the human genome is ahead of schedule, thanks in part to new tools that have accelerated DNA sequencing and reduced its cost. (The DOE sequencing team can generate more data in 8 days now than it did in all of 1998, its first full year of operation.) One such tool developed in the mid-1990s is an enzyme, a type of DNA polymerase. Polymerases, which in their natural form help cells replicate genetic material, are used in sequencing to incorporate fluorescent tags into DNA to identify the locations of specific chemical units. Naturally occurring polymerases tend to reject fluorescent labels. But Stanley Tabor and Charles Richardson of Harvard Medical School, with Office of Science support, applied fundamental discoveries of the structure and mechanisms of polymerases to create a new DNA polymerase, in which a single chemical change eliminated the bias against fluorescent bases—thereby producing more usable data than was generated previously. This discovery, along with other new knowledge about organisms living in extreme environments, was used by a company to engineer a polymerase that both incorporates the labels and has the thermostability needed for sequencing.

Scientific Impact: Tabor and Richardson's discovery solved a long-standing problem in genetic research. The commercial enzyme, ThermoSequenase, now used by all DNA sequencing centers, has improved the quality of sequencing data and reduced the costs.

Social Impact: ThermoSequenase has captured a very large share of the DNA-polymerase world market, now more than $350 million and growing. It is among the tools used in decoding the human genome, recently completed in "working draft" form, which is expected to lead to new understanding of, and treatments for, human diseases.

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Doublié, S., Tabor, S., Long, A. M., Richardson, C. C. and Ellenberger, T. (1998) "Crystal structure of a bacteriophage T7 DNA replication complex at 2.2 Å resolution," *Nature* 39, 251-258.

Patents: Tabor, S., and Richardson, C. C. (1997) DNA polymerases with a modified nucleotide binding site for DNA sequencing. U. S. patent number 5,614,365.

Tabor, S., and Richardson, C. C. (1997) Method of sequencing based on uniform band intensities. U. S. patent number 5,674,716.

SC-Funding Office: Office of Biological and Environmental Research

6.8 Tiny Capillaries Have Giant Impact on DNA Sequencing

Electrophoresis

Richard Mathies

Advances in sequencing the human and other genomes required new, faster and cheaper techniques for automating the process. Fundamental research on polymers led to development in the 1990s of long, water-soluble polymers that could be pumped into minute capillaries yet remain viscous at the high voltages required for sequencing. Parallel developments were greatly improved reporting fluors for DNA and systems for DNA readouts from bundled capillaries.

Scientific Impact: The DNA sequencing using capillary electrophoresis allowed much greater automation, with much higher throughputs and further cost reductions due to reduced reagent use. The techniques developed in the project resulted in the commercialization of the two types of DNA sequencing machines now used in all major DNA sequencing laboratories.

Social Impact: Automation of electrophoresis greatly increased the speed at which we were able to sequence the human genome, and made this research affordable for medical and other uses.

Reference: Carrilho, Emanuel, Marie C. Ruiz-Martinez, Jan Berka, Igor Smirnov, Wolfgang Goetzinger, Arthur W. Miller, David Brady, and Barry L. Karger. 1996. "Rapid DNA Sequencing of More Than 1000 Bases per Run by Capillary Electrophoresis Using Replaceable Linear Polyacrylamide Solutions," *Analytical Chemistry* 66:3305-3313.

Liu, Shaorong, Yining Shi, William W. Ja, and Richard A. Mathies. 1999. "Optimization of High-Speed DNA Sequencing on Microfabricated Capillary Electrophoresis Channels," *Analytical Chemistry* 71:566-573.

SC-Funding Office: Office of Biological and Environmental Research

6.9 "Painting" Chromosomes for Quick and Easy Analysis

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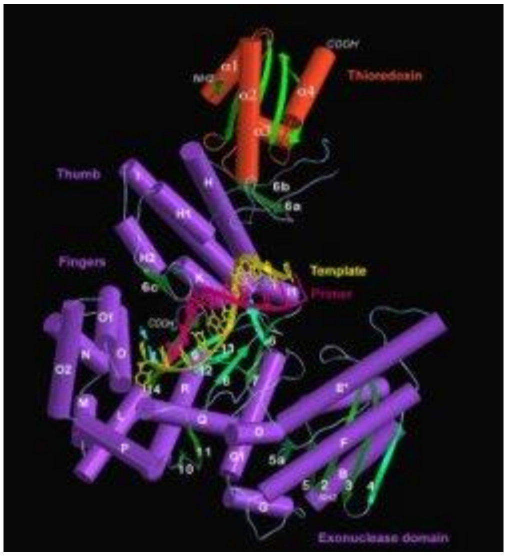
6.10 Putting a Virus to Practical Use



T7 DNA Polymerase Structure

Electron micrograph of the bacteriophage T7.

A virus is usually viewed as a problem, but T7 turned out to be useful, even valuable. In 1982, Brookhaven National Laboratory scientists, led by biologist William Studier, finished determining the DNA sequence of T7, a bacteriophage (bacteria-eating virus) that had the longest DNA sequence then known. When T7 invades a host cell, it makes proteins that turn off the host genes and turn on T7 genes. Researchers correlated the genetic map with T7's protein production, thereby acquiring a detailed understanding of how such viruses control their own replication. Studier and colleagues used this knowledge to develop a series of T7-based protein expression systems in which the gene of interest is silent until its expression is induced by a simple chemical trigger added to the culture. The protein products then are produced in abundance, even if the host cells eventually fail. In addition, the target genes can be engineered so that the proteins produced carry "affinity tags" enabling their rapid purification.

Scientific Impact: Widely used in molecular genetics and biotechnology, T7 protein expressions systems are noted for their reliability and adaptability. Even gene products that are difficult to express (e.g., toxic products) can be successfully produced using these systems.

Social Impact: The T7 system has become one of the most commercially successful, biologically based systems for producing large quantities of specific proteins. Even basic research using these systems sometimes has a practical impact, as in the case of recent work on a protein associated with Lyme disease that led to the development of improved vaccines.

References: Studier, F.W. and B.A. Moffatt, "Use of bacteriophage T7 RNA polymerase to direct selective high-level expression of cloned genes," *J. Mol. Biol.* 189: 113-130 (1986).

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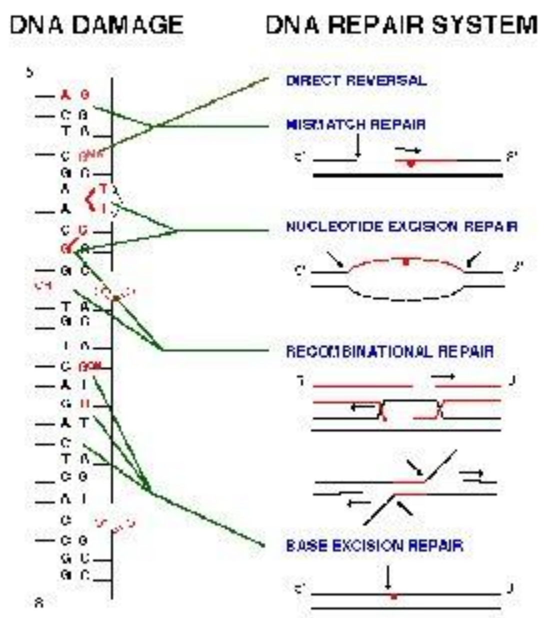
SC-Funding Office: Office of Biological and Environmental Research

6.11 Unraveling the Role of DNA Repair



Schematic of different mechanisms of DNA damage.

Ionizing radiation, chemicals, and other agents can result in genetic damage, which, if not repaired, can lead to diseases such as cancer. Fortunately, a system of genes directs the production of sensitive DNA repair enzymes, which monitor for genetic damage and fix most errors. The role of DNA repair processes in fixing genetic damage, as well as the role of genetically impaired repair mechanisms in cancer, were first discovered by investigators funded by predecessors to the Office of Science in the 1960s. More recently at Lawrence Livermore, Los Alamos, and Lawrence Berkeley national laboratories, researchers have cloned and studied a number of crucial DNA repair genes. A clear picture is emerging that unrepaired DNA damage is the culprit in the long-term consequences of radiation exposure. Scientists now see that X-rays, ultraviolet light, and cancer-causing chemicals work in similar ways in disabling the natural DNA repair mechanisms. A team at Lawrence Berkeley demonstrated a strong correlation between the inability to repair oxidative damage to DNA and severe developmental failure and early death in a hereditary condition called Cockayne's syndrome.

Scientific Impact: Research on DNA repair helps scientists better understand biological processes, from the microscale (e.g., cell death) to the macroscale (e.g., evolution). So central is the role of DNA repair that in 1994, *Science* magazine designated the entire class of DNA repair enzymes as "Molecule of the Year."

Social Impact: By explaining how DNA repair processes can go awry, scientists contribute to sound policymaking on environmental hazards. This research also could lead to medical and pharmaceutical treatments for repair-deficiency disorders, implicated in conditions ranging from cancer to aging.

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SC-Funding Office: Office of Biological and Environmental Research

6.12 Of Mice and Men

Fat Agouti and normal mice.

Scanning electron micrograph of deoxygenated red blood cells from transgenic mouse exhibiting typical sickle-cell characteristics.

Although they differ dramatically in size and appearance, mice and humans are very similar genetically. For this and other reasons, the mouse is the most widely used model for studies of human gene function. Many such studies have been funded by the Office of Science and predecessor agencies. In the 1940s, Bill and Lee Russell started a mouse genetics program at Oak Ridge National Laboratory, where they set up the "mouse house," which became one of the world's largest colonies of experimental mice (it houses some 70,000 mice today). Their studies of genetic mutations led to a number of discoveries, as in 1979, when Bill Russell found that the laboratory chemical ethylnitrosourea is the most potent mutagen ever tested in mice, making it a useful research tool. In 1992, Richard Woychik and colleagues at Oak Ridge showed that a long-studied gene for a color mutation of the mouse coat, known as the Agouti gene, is related to a human gene that contributes to obesity and insulin-dependent diabetes. More recently, Chris Paszty and Edward Rubin of Lawrence Berkeley National Laboratory worked with other scientists to genetically engineer the first strain of mice to mimic fully all the symptoms of human sickle cell disease, thus offering a way to test experimental treatments.

Scientific Impact: Research on mice has contributed significantly to the field of mammalian mutagenesis, and thus to the practice of genetic risk assessment. For example, ethylnitrosourea has become a standard tool for studying gene function and mechanisms of mutagenesis.

Social Impact: Based on mouse studies, scientists have developed new leads to treatments for obesity, insulin-independent diabetes, Down syndrome, liver cancer, kidney disease, leukemia, sickle-cell disease, and many other conditions. In addition, research on genetic mutations in mice led to reductions in permissible levels of occupational exposure to radiation.

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Russell, W. L., E. M. Kelly, P. R. Hunsicker, J. W. Bangham, S. C. Maddux, and E. L. Phipps, "Specific-locus test shows ethylnitrosourea to be the most potent mutagen in the mouse," *Proc. Natl. Acad. Sci*. USA 76:5818-5819 (1979).

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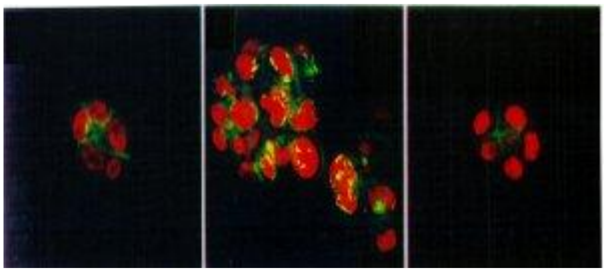
SC-Funding Office: Office of Biological and Environmental Research

6.13 The Role of the Extracellular Matrix in Cancer



Normal breast cells organized in three dimension (left), breast tumor cells unable to form organized tissue-like structure (middle), reversion of tumor cells to near normal appearance by extracellular matrix (right).

The extracellular matrix (ECM), the network of proteins surrounding cells in the body, long was believed to function mainly as inert scaffolding for tissue. But in the early 1980s, Mina Bissell of Lawrence Berkeley National Laboratory proposed that the ECM is a key "signaling molecule" crucial for the normal functioning of cells. That is, the ECM is one of the environmental factors (along with hormones) that communicate with a cell nucleus, modifying nuclear structures and leading to selective gene expression. Bissell's theory implied that alterations in the ECM or cellular responses to it could lead to malignancy, a radical idea at the time. Her experiments showed that in standard cultures, cancerous breast cells grew at the same rate and took on the same flat appearance as healthy breast cells. But when ECM was added to the culture, the healthy cells once again became plump and round and began secreting milk, whereas the cancerous cells grew wildly into a tumorous mass. Bissell was among the first to connect the regulation of cell growth and development with the cell's environment.

Scientific Impact: The ECM theory has steadily gained scientific acceptance and yielded a growing volume of knowledge about both normal and breast cancer cells. Bissell?s work has greatly influenced cell biology, a field in which cells are studied as living entities that take on specialized functions, organize into communities, and interact with their environment.

Social Impact: The new understanding of the ECM provides information essential to the diagnosis and successful treatment of cancer. This work suggests that, even after cancer genes have been activated and lesions have formed, it may still be possible to reverse the process and restore the cells to normal appearance and function.

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SC-Funding Office: Office of Biological and Environmental Research

6.14 New Tools for Structural Biology Research

State-of-the-art beam lines, instrumentation, techniques, and software for investigating macromolecular structures have been developed by biologists at the Office of Science's four synchrotron radiation facilities, in cooperation with the National Institutes of Health and public and private consortia. These facilities make possible new science, from basic biology to immunology to studies on DNA damage and repair. As an example, more than 600 biologists from universities, pharmaceutical companies, and other national laboratories used seven experimental stations at Brookhaven National Laboratory in the past year to study biological molecules using a technique called X-ray crystallography. The work requires sophisticated detectors to capture the X-rays scattered by atoms in crystallized molecules, and advanced computer software to translate those data into a finished images of molecules. Collectively, the four facilities served about 2,000 unique users in fiscal year 2000, providing high operational efficiency and, in many cases, remote access and automated data collection and reduction.

Scientific Impact: These resources provide the foundation for new initiatives in structural genomics. Recently, studies have shown structures of key components of the infectious agents involved in such diseases as tuberculosis, Lyme disease and AIDS as well as proteins that play central roles in cystic fibrosis and similar disorders."

Social Impact: These state-of-the-art facilities will help scientists from all over the world discover new biological information about the human body, disease agents, and crop plants. Research results may help pharmaceutical and agrichemical companies develop new pharmaceuticals and agricultural products.

References: Chang, G.; Spencer, R.H.; Lee,A.T.; Barclay, M.T.; Rees,D.C., "Structure of the MscL Homolog from Mycobacterium tuberculosis: A Gated Mechanosensitive Ion Channel," *Science*, 282, 2220-2226 (1998).

Kumanan, D. Eswaramoorthy, S.; Luft, B.J.; Koide, S.; Dunn, J.J.; Lawson, C.L.; Swaminathan, S., "Crystal structure of outer surface protein C (OspC) from the Lyme disease spirochete, Borrelia burgdorferi." *EMBO Journal*, 20, 971-978 (2001).

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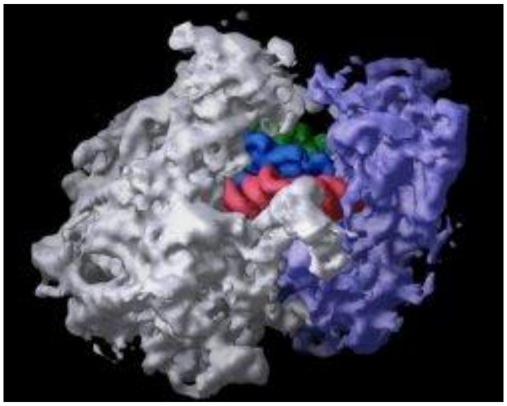
SC-Funding Office: Office of Biological and Environmental Research

6.15 The Structure of Nature's "Molecular Machines"



Space filled model of a 70S ribosome.

Now that scientists have determined most of the sequence of chemical units in the human genome, a next step is to unravel the mechanisms directed by the genetic code. Scientists got a close look at some of these mechanisms recently by using synchrotron light sources to make images of RNA polymerase, both subunits of the ribosome, and the full ribosome. These "molecular machines" read the genetic message and accurately make the proteins that form the structures and perform the functions of living organisms. These assemblies have been the subjects of intense study for 30 years, but only recently have advances in synchrotron technology, crystal sample quality, experimental methods, and computational approaches enabled near-atomic resolution of their structures. The new images reveal in minute detail how DNA is unwound, how a message (mRNA) is created with the help of RNA polymerase, how this message is read by a ribosome, and how the ribosome synthesizes protein. The image of the complete ribosome was named by *Science* magazine as one of the top 10 scientific breakthroughs of 1999. The work was performed at Lawrence Berkeley National Laboratory, Argonne National Laboratory, and Stanford Synchrotron Radiation Laboratory.

Scientific Impact: These images demonstrated that there is much more to ribosomal structures than previously thought. They also helped bolster the theory that RNA molecules were among life's first, with proteins emerging at a later time.

Social Impact: Studies of this type are expected to help lay the groundwork for improved drug design, faster diagnosis of disease, and better disease prevention and treatment methods.

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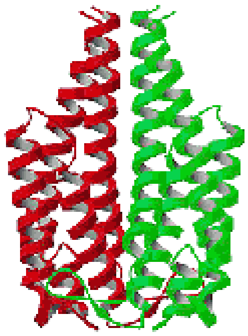
SC-Funding Office: Office of Biological and Environmental Research

6.16 Studies of Protein Structure Help Fight Lyme Disease



Structure of OspA surface protein from Lyme disease bacterium.

Lyme disease, a bacterial infection transmitted to humans through a tick bite, causes rashes, fever, arthritis, and nerve damage and is an increasing concern in the northeastern United States. Although treatable with antibiotics, Lyme disease can be difficult to diagnose, and untreated infections can progress to severe complications. Accordingly, scientists have sought to design a safe, effective vaccine. The original Lyme disease vaccine often failed, for reasons that were unclear until Cathy Lawson and John Dunn at Brookhaven National Laboratory explained why. Using intense X-rays at the National Synchrotron Light Source, they identified variations in the structure of a key surface protein, OspA, from the bacterium that causes Lyme disease. The OspA structure contains several regions that vary among different strains of the bacterium and other regions that are invariant. The original vaccine was developed against a variant region from only one strain, so it did not protect against other strains. Continuing Brookhaven research on other Lyme disease proteins could lead to further improvements in vaccines.

Scientific Impact: The structural model of OspA, showing the exact locations where different strains of the bacterium vary, helped researchers quickly solve an urgent problem. This work also demonstrated the value of the latest synchrotron technologies.

Social Impact: The second-generation vaccines—protecting against many strains of the bacterium—have been commercialized and are much more effective than earlier versions in inducing general immunity to, and preventing, Lyme disease in people. Brookhaven research on other Lyme disease proteins has led to the development of a rapid, highly accurate diagnostic test for the disease, recently granted approval by the Food and Drug Administration.

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Kumanan, D. Eswaramoorthy, S.; Luft, B.J.; Koide4, S.; Dunn, J.J.; Lawson, C.L.; Swaminathan, S., "Crystal structure of outer surface protein C (OspC) from the Lyme disease spirochete, Borrelia burgdorferi," *EMBO Journal*, 20, 971-978 (2001).

SC-Funding Office: Office of Biological and Environmental Research

6.17 Accelerating the Study of Proteins

11.5 Tesla Fourier transform ion cyclotron resonance mass spectrometer at the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory

With the completion of DNA sequences from a rapidly growing number of organisms, scientists now want to identify and characterize all of the genes and their protein products. Measurements of protein production, for example, could provide new insights into the molecular nature of disease and many other biological processes. Protein studies generally proceed slowly, but Richard Smith of Pacific Northwest National Laboratory recently developed an instrument that greatly accelerates such research. The innovation involves a unique type of mass spectrometry—orders of magnitude more informative and sensitive than previous systems—operating in a rapid, high-volume mode to simultaneously study all of an organism's proteins, or the proteome. (The proteome is the entire complement of proteins that can be expressed by a particular cell, organism, or tissue.) No other existing technology can perform this task. A pilot demonstration in 2000 focusing on an important microorganism generated much more data than was obtained in all previous studies, and in much less time and at much lower cost.

Scientific Impact: This instrument will have a broad impact on biological research, especially proteomics, the study of the protein complement expressed at a given time or under a specific set of environmental conditions. It will enable direct, quantitative comparisons of the proteins expressed under different conditions, a key question in understanding how biological systems work and respond to their environments.

Social Impact: The capability to make these rapid, data-rich measurements of proteomes will have enormous and almost immediate impacts on many areas of biomedical research. The new understanding developed as a result may broadly influence the human condition, including the life span and quality of life.

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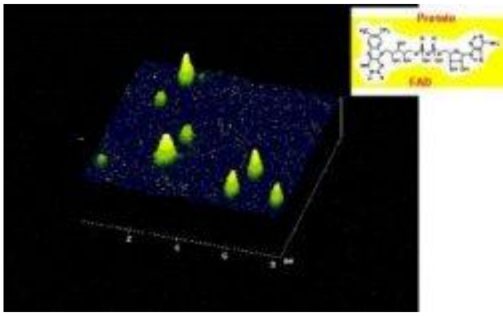
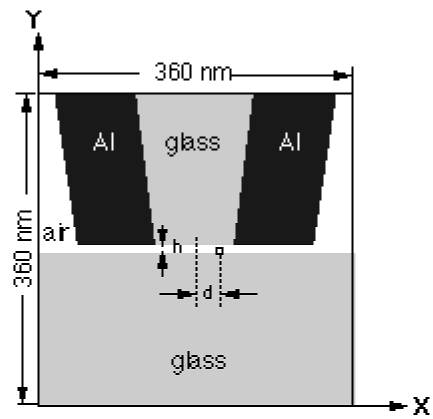
SC-Funding Office: Office of Biological and Environmental Research

6.18 Optical Probes for Imaging Single Molecules





Fluorescent image of single molecules of cholesterol oxidase and probe tip used to image single molecules.

With conventional optics, scientists can image an area no smaller than one-half of the wavelength of light being used. But scientists at Pacific Northwest National Laboratory found a way to deliver light energy to areas much smaller than its wavelength. During the 1990s, Sunney Xie, Peter Lu, and coworkers developed a near-field optical imaging technique that provides spectral information about the interaction of single molecules with surfaces, making it possible to study, for example, the dynamic behaviors of proteins in real time on the microsecond time scale. Similar research tools, such as optical tweezers and atomic force microscopy, provide spatial and structural information with sub-nanometer resolution, but not the spectral information that is vital for understanding the chemical properties of molecules and other sub-nanometer structures. Near-field optical probes enable the study of individual molecules in their own environments, providing new insights into the nature of reactions in natural systems.

Scientific Impact: This technique has proven very helpful for studying reactions of biological molecules and other condensed phase processes in natural systems. Many such processes cannot be understood without some means, such as optical probes, of resolving the effects of time- and geometry-dependent perturbations.

Social Impact: This instrumentation is being used to elucidate the biological effects of chemical and radiation exposure and thus may help improve human health. It also may contribute to new ways of using natural enzymes in the remediation of contaminated soils and groundwater, and to the development of nanoscale electro-optical devices.

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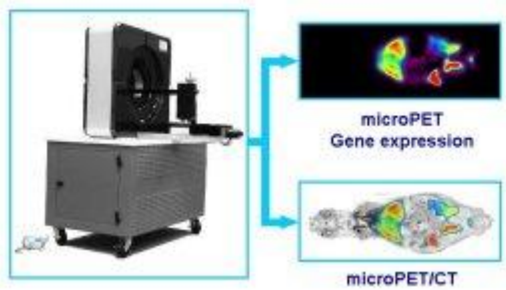
SC-Funding Office: Office of Biological and Environmental Research

6.19 MicroPET Enhances Studies of Small Animals



A miniature PET scanner, the "microPET," for imaging mice enables scientists to develop new ways to provide real time images of the molecules that transform normal cells to diseased cells in a living mouse. The microPET mouse image shows an example of how BER scientists at UCLA watch the genome of cells at work in the living mouse.

Positron emission tomography (PET), a tool for imaging the chemistry and biology of the living human body by monitoring ingested tracer molecules, is now a standard method for studying the metabolism of the brain, the heart, and cancer. PET is based on pioneering advances by the Office of Science and predecessor agencies in particle accelerators, biological radiotracer molecules, photodetectors, and high-speed computers. Recently, PET technology was reengineered by scientists at the University of California-Los Angeles to make a miniaturized version for imaging small animals. Developed with Office of Science support, MicroPET is a noninvasive system that eliminates the need for biopsies and thereby extends an animal's life. It allows serial and longitudinal studies to be performed on the same living animal, enabling researchers to follow a single animal over time and monitor the effects of interventions on disease progression and outcome. MicroPET will be particularly valuable for studying genetically modified animals that exhibit high variability or are unique or valuable. Demand for this technology has been created by accelerated progress in decoding the human genome, development of transgenic mice, and rapid proliferation of small animal models of human disease.

Scientific Impact: More than 260 centers worldwide (70 in the United States) use PET scanners, including one at Lawrence Berkeley National Laboratory with the world's highest resolution. There are eight operational MicroPET systems, as well as numerous additional orders; these systems are expected to significantly improve the results and reduce the costs of research on animal models for human disease.

Social Impact: PET scanning provides improved diagnosis of disorders such as epilepsy, Alzheimer's disease, Parkinson's disease, cardiovascular diseases, and many cancers. Research using MicroPET will enabled the analysis of genetic manipulations, biological transformations, and progression of disease in living animals as a means of gaining insight into these processes in humans.

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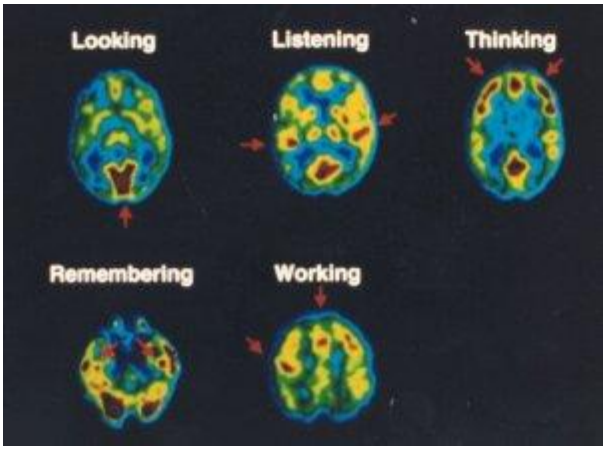
SC-Funding Office: Office of Biological and Environmental Research

6.20 Mapping Human Brain Function



PET scans show different patterns of glucose (sugar) metabolism related to performing various mental tasks.

Many mysteries of the human brain have been unraveled by positron emission tomography (PET), an imaging tool used worldwide to diagnose cancer and heart disease and perform scientific studies. The development and usefulness of PET—which offers a millionfold greater sensitivity than other techniques for studying regional metabolism and neuroreceptor activity in the brain and other tissues—rests on a number of advances made with Office of Science support. Much of the credit is due to Alfred P. Wolf, a chemist at Brookhaven National Laboratory known as the father of organic radiochemistry, a field that links medicine and chemistry. In 1976, Wolf and colleagues developed and used a radiotracer called 18-fluorodeoxyglucose (a combination of the short-lived radioactive element fluorine-18 and a sugar, glucose) to generate the first functional map of the human brain at work. When a radiotracer is injected into the body, its signal is picked up by PET equipment. Glucose is virtually the only energy source for the brain, so images of the location of 18-FDG provide a signature or map of brain function. This development enabled scientists to see, for the first time, regions of the human brain "lit up" in response to stimuli such as looking, listening, and remembering.

Scientific Impact: The development of 18-FDG, as well as improvements in image reconstruction algorithms and nuclear detector technologies, enabled widespread use of PET by the mid-1980s. Scientific uses include studies of human metabolism, brain activation and function, addiction, and mental illness. Radiotracers have also been used to track the movement of air in the atmosphere and study basic chemical processes.

Social Impact: Wolf's work laid the foundation for imaging procedures now used in hospitals worldwide to diagnose disease, saving thousands of lives each year. These developments opened new vistas for mapping of human brain function in schizophrenia, Alzheimer's disease, stroke, addiction, and other psychiatric and neurological disorders.

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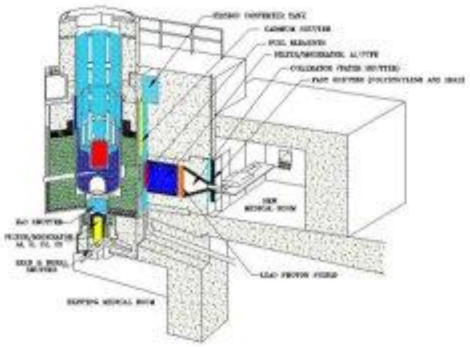
SC-Funding Office: Office of Biological and Environmental Research

6.21 Improving Neutron Beams for Cancer Treatment



The MIT Fission Converter first began operation in June of 2000. It delivers a high quality epithermal beam of about 1010 neutrons/cm^{2}sec, making it ideal for use in Boron Neutron Capture Therapy. (Click here to see larger version.)

Beams of neutrons long have been used in scientific experiments, but recently, for the first time, a novel type of neutron beam was generated for use in a medical reactor. The innovation by Otto K. Harling of Massachusetts Institute of Technology involved the adaptation of existing nuclear fission converter technology. The Office of Science supported the detailed scientific and engineering design needed to put the concept to practical medical use. The new technology was used to upgrade MIT's medical reactor for studies of boron neutron capture therapy (BNCT), first attempted in the United States in the 1950s at Brookhaven National Laboratory. Those early efforts were unsuccessful, but the new MIT beam is epithermal (intermediate energy) and can penetrate more deeply than the low-energy neutrons used in the past, thereby eliminating the need for surgery. The latest BNCT technology also incorporates an improved boron-containing drug and rapid, accurate boron analysis technology. In BNCT, the patient consumes a drink containing boron, which is taken up by tumor cells. The tumor then is irradiated with a neutron beam, causing the boron to split into two highly energetic particles that destroy the tumor cells while largely sparing adjacent healthy cells.

Scientific Impact: This work demonstrates the value of long-term interdisciplinary and inter-institutional efforts to design, develop, and field innovative technology. The improved neutron beam has helped make MIT's medical reactor the most advanced epithermal neutron source in the world for cancer treatment.

Social Impact: Preliminary trials of BNCT therapy supported by the Office of Science have shown promise for the treatment of malignant melanomas. The National Institutes of Health is considering but has not yet approved clinical trials, for which the MIT facility is the only suitable site in the United States.

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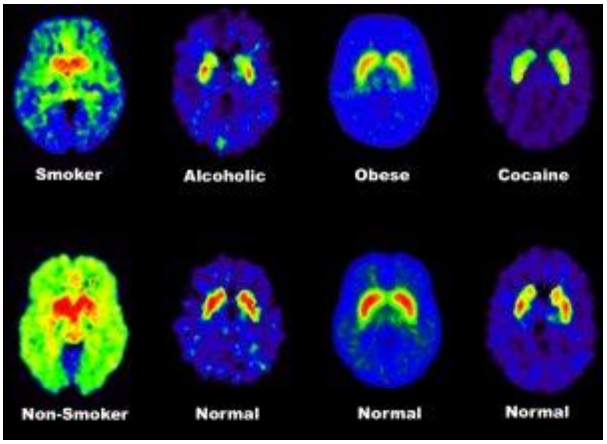
SC-Funding Office: Office of Biological and Environmental Research

6.22 The Biochemistry of Human Addiction



PET brain scans reveal chemical differences in the brain between addicts and non-addicts. The normal images in the bottom row come from non-addicts; the abnormal images in the top row come from patients with addiction disorders.

Dopamine, a brain chemical linked to pleasure and elation, also has a dark side—a link to addiction. This link has been explored in detail by Nora Volkow of Brookhaven National Laboratory, a world leader in addiction research. Volkow has shown that that addicts have fewer than average dopamine receptors in their brains, so that weaker dopamine signals are sent between cells, and life naturally has less joy. Addicts thus are encouraged to derive pleasure from dopamine-stimulant drugs, such as alcohol, cocaine, and nicotine. This cycle was first identified in 1990, when Volkow and coworkers showed that cocaine addiction blunts the dopamine signaling system. Using positron emission tomography, an imaging technique developed with Office of Science support, they determined the critical biochemical changes and where they occur in the brain in response to addictive drugs. These studies demonstrated that addictions are associated with high levels of dopamine in a pleasure center in the brain. The findings have been proven again and again in studies of addictions to drugs and food/overeating. It is not yet clear whether a preexisting dopamine abnormality leads to addiction, or vice versa.

Scientific Impact: This work may have uncovered a common biochemical pathway for addiction. The findings also opened up new research areas, including efforts at Brookhaven and elsewhere to find dopamine-blocking agents that could be given to addicts to make drugs less alluring, and Volkow's studies of the link between addiction and an area of the brain associated with higher thinking and obsessive-compulsive behavior.

Social Impact: Volkow's work has led the way in debunking the idea that sheer willpower is a cure for addictions. Understanding of the molecular mechanisms underlying drug addiction could lead to new approaches for interrupting addictive behavior and have lasting impacts on how society copes with this public health problem.

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SC-Funding Office: Office of Biological and Environmental Research

6.23 Observing Chemical Changes in Living Cells

The combined OM/MRM microscope. The microscope consists of a bottom-loading optical microscope and a top-loading MR microscope; both inserted into a c vertical bore 11.7 Tesla magnet.

Just a few years ago, scientists were unable to observe chemical changes within normal living cells, because the analytical methods destroyed or modified the cells. But a new method surmounts these problems. Scientists from Pacific Northwest National Laboratory and the Massachusetts Institute of Technology recently developed a system making it possible, for the first time, to simultaneously image "live" cellular systems using both optical microscopy and nuclear magnetic resonance (NMR) microscopy. The system combines new image contrast techniques, enhanced specificity to cellular events, and reduced NMR microscopy measurement times. The NMR imager works like a magnetic resonance imaging unit at a modern hospital, except that it examines much smaller collections of cells, down to a single cell and its nucleus. Furthermore, the new microscope reveals information about a cell's chemical composition and allows scientists to monitor changes in both the shape and chemical Back to Decades of Discovery home of the cells as they occur.

Scientific Impact: This noninvasive technique will enable scientists to monitor how live cells respond as they are exposed to environmental changes, such as heat, chemicals, and radiation. Scientists will also be able to see what happens when cells are exposed to multiple contaminants at the same time, and, ultimately, to relate these responses to large-scale effects.

Social Impact: This new capability will greatly enhance understanding of the connection between environmental exposures and human health problems. Studies of cellular changes in real time will help explain how cells succeed or fail in fighting off diseases, and enable practitioners to track healthy cells that become cancerous or diseased cells undergoing treatment.

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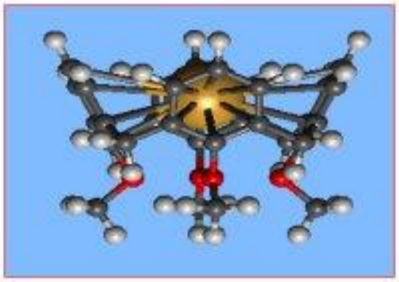
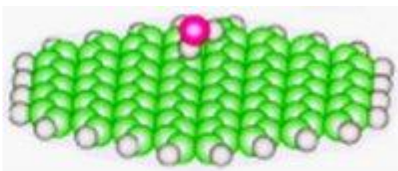
SC-Funding Office: Office of Biological and Environmental Research

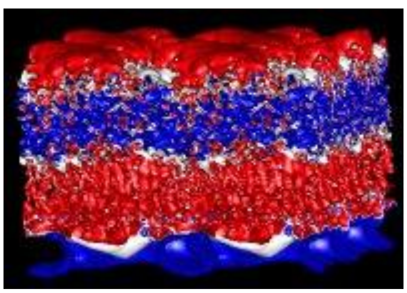
6.24 Modeling and Simulating Environmental Problems



Model for binding of water to a model of single-layer graphite.



Predicted structure for cesium cation binding to a tetramethoxycalix[4]arene.



Electrostatic potential of the lipopolysaccharide membrane of a microorganism.

To model and simulate major environmental problems, scientists need more than the most powerful computers. They also need software algorithms that express the fundamental physics involved in entirely new ways, appropriate to parallel processing. Software of this type was developed recently by computational scientists, applied mathematicians, and theoretical chemists from the Pacific Northwest National Laboratory. Northwest Computational Chemistry Software (NWChem) is an advanced molecular modeling package featuring major design improvements over traditional codes, including new algorithms for computational chemistry and the high-level data and control structures needed to make parallel programs easier to write, maintain, extend, and use on a broad range of parallel computers. NWChem provides many methods for computing the properties of molecular systems by using quantum mechanics based on either molecular orbital theory or density functional theory. The software also can perform classical molecular dynamics and free-energy simulations of macromolecular and solution systems. For the first time, these approaches can be readily combined to perform mixed quantum mechanics and molecular dynamics simulations.

Scientific Impact: Developed in the mid-1990's at PNNL's Environmental Molecular Sciences Laboratory (EMSL), NWChem has been distributed to more than 300 sites worldwide, including most federal supercomputing centers and many universities. Scientists are using it to run modeling and simulation studies of DOE's environmental problems and other subjects, from combustion to petrochemical zeolite catalysts.

Social Impact: Studies using this software are addressing health and environmental issues and thus may eventually affect everyday life. NWChem has been used to study, for example, protein models for drug design, DNA chips, catalysts for the petroleum industry, geochemical surfaces for bioremediation, and atmospheric pollutants including aerosols.

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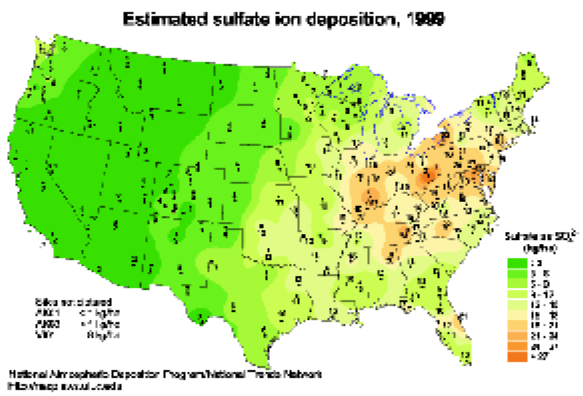
SC-Funding Office: Office of Biological and Environmental Research

6.25 Discovering the Processes of Acid Rain



Estimated sulfate ion deposition, 1999.

Acid rain is created when sulfur and nitrogen emissions from industrial processes and cars dissolve in water droplets in clouds and form sulfuric and nitric acids. Scientists at several national laboratories were the first to uncover the detailed chemical and atmospheric processes that convert these emissions to acids, which then are deposited on the ground in both dry and wet forms. They established that inorganic sulfur and nitrogen species are the major anthropogenic contributors to acid deposition and that dry deposition can account for a third to a half of the total input, depending on location. They also documented the importance of adsorption-desorption properties in soils, especially the role of hydrous oxide coatings on soil particles, as a buffering mechanism that reduces the transport of sulfate deposited from the atmosphere into surface waters. These discoveries led to the development of models that provide realistic simulations of acid deposition scenarios. The work was performed at Argonne, Brookhaven, Oak Ridge, and Pacific Northwest national laboratories.

Scientific Impact: This research contributed to understanding of the processes that both generate acidic deposition and determine the extent of its effects on terrestrial and aquatic ecosystems. Before this work began in the late 1970s, very little was known about the mechanisms producing acid rain; by the early 1990s, the scientific questions were resolved sufficiently that the processes could be modeled.

Social Impact: The acid deposition models enabled by these discoveries were essential for the development of pollution control measures and pollution prevention strategies. The scientific and modeling advances also led to a political consensus on the actions needed; releases of sulfur dioxide and nitrogen oxides have been cut drastically in recent decades because of new laws.

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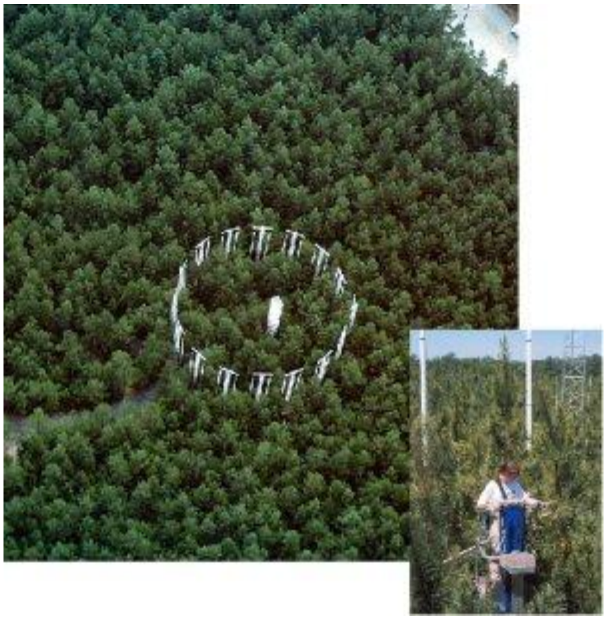
SC-Funding Office: Office of Biological and Environmental Research

6.26 Predicting Effects of Elevated Carbon Dioxide



Free Air CO2 Experiment (FACE) predicts forest ecosystem response to elevated carbon dioxide. Scientist is measuring photosynthesis of pine trees, and the experiment provides other data on tree growth and carbon sequestration.

Increasing concentrations of carbon dioxide (CO2) in the atmosphere, resulting from fossil-fuel combustion and other sources, are an international concern because of the possible effects on climate. Predictions of climate impacts will be most reliable if based on experiments that mimic real world conditions, meaning they are conducted in open-air field sites rather than greenhouses or other enclosures. These types of long-term, controlled field studies in a number of different ecosystems have been made possible by the development of the Free-Air CO2 Enrichment (FACE) methodology at Brookhaven National Laboratory. The unique FACE facilities and techniques enable scientists to increase the concentration of trace gases such as CO2 in the atmosphere above the ground in a controlled way in intact ecosystems, and to study plant response to the altered conditions. Several FACE facilities are operating around the world. Research supported by the Office of Science has revealed differential responses among species within a single ecosystem; increasing CO2 causes some plants to grow faster and larger and to use less water.

Scientific Impact: The FACE approach gives many biologists access to a large facility that encompasses hundreds of individual plants in an intact ecosystem. This is an economical way to build an understanding of how a particular ecosystem will respond to rising levels of CO2, information that is critical to understanding and predicting overall environmental impacts.

Social Impact: FACE studies will help society plan for the predicted CO2-rich atmosphere of the future. For instance, results from a FACE facility operated by Brookhaven in North Carolina showed that, in 50 years, if forests worldwide were to grow 25 percent faster than they do now, then plant life could serve as a "sink" for about half the expected CO2 emissions from fossil-fuel combustion.

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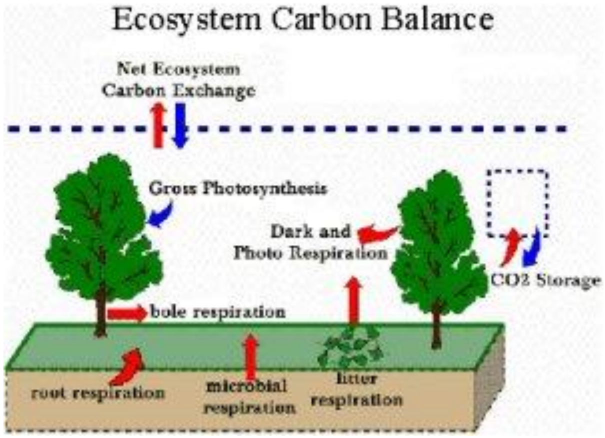
SC-Funding Office: Office of Biological and Environmental Research

6.27 Clues to the Location of the Missing Carbon Dioxide



The flux of carbon dioxide is measured between the atmosphere above the plant canopy on the trees of a forest ecosystem. In the vast majority of AmeriFlux sites the flux is into the trees resulting in the forest becoming a significant sink for excess CO2 from the atmosphere.

Major changes are occurring in the chemical composition of the atmosphere, most notably an increase in carbon dioxide (CO2) concentration. A fuller understanding of the global carbon cycle is needed so that future changes can be predicted and policies can be developed on energy use. Roughly half of the CO2 released by human activities remains in the atmosphere; scientists do not know whether the missing half is sequestered in the deep oceans, soils, or plant biomass. Recently, some clues have been found. Over the past 10 years, university researchers supported by the Office of Science have discovered that net carbon sequestration by forests along a north-south climate gradient, ranging from Canada to the southeastern United States, increases with rising temperature. This discovery was made using the AmeriFlux facilities, a network of approximately 25 research sites in a large variety of ecosystems in North, Central, and South America. At each site, continuous measurements are made of the turbulent exchange of CO2, water vapor, and energy between the atmosphere and terrestrial biosphere.

Scientific Impact: AmeriFlux data will help scientists understand why the sequestration of carbon varies among different types of terrestrial ecosystems, and how their capacity to sequester carbon might change in response to human-induced and natural changes in climatic conditions. The data also will be used to test elements of global climate and ecosystem models.

Social Impact: This work will help society make wise decisions about land use and land management, such as whether forests will be protected and managed to remain an important net sink for atmospheric CO2 or are converted to other land uses that are a smaller net sink or a net source of CO2. Possible adverse effects of elevated CO2 levels include global warming.

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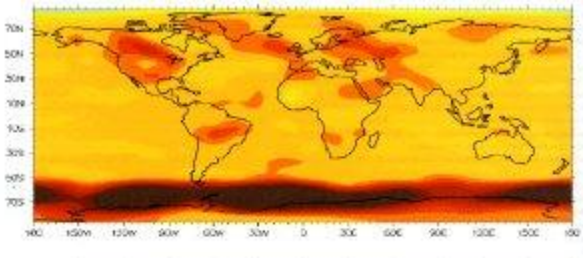
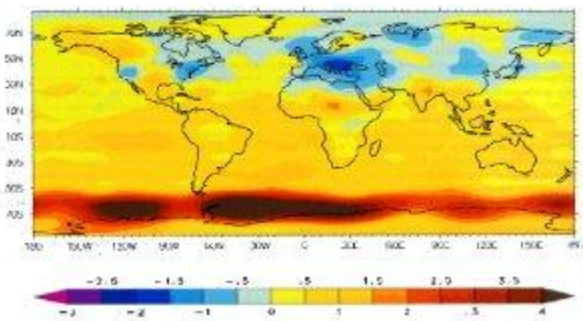
SC-Funding Office: Office of Biological and Environmental Research

6.28 Human Effects on Global Warming



Greenhouse gas forcing only.



Greenhouse gas and sulfate aerosol forcing.

By themselves, droplets of sulfuric acid resulting from the burning of fossil fuels are of little consequence. But vast numbers of them form an aerosol haze that moderates and obscures the "greenhouse effect" caused by heat-trapping gases. In 1995, Benjamin Santer of Lawrence Livermore National Laboratory was the first to quantify and explain the link between fossil fuel emissions and climate change, including the role of greenhouse gases and aerosol particles. Using a statistical pattern detection method, Santer and colleagues reviewed records of the past century and identified the anthropogenic "fingerprint" of climate change that took into account the confounding effects of natural variations. This work explored the implications of earlier research by Karl Taylor and Joyce Penner of Lawrence Livermore, who showed that sulfate aerosols have strong local cooling effects and significantly modify the climate change pattern associated with greenhouse gases alone. Santer's studies demonstrated that the inclusion of sulfate aerosol effects helped to bring model simulations in closer statistical agreement with observations, and that this correlation is improved further by the inclusion of other relevant factors, such as ozone depletion and the effects of volcanic eruptions.

Scientific Impact: Most climate modeling centers now emulate the work of these scientists by incorporating a sulfate chemistry model within an atmospheric/ocean climate model. The statistical technique of fingerprinting has since become the foundation for more complex methods of separating signals from noise in climate records.

Social Impact: Santer's studies provided hard evidence that human activities have global-scale consequences. The internationally acclaimed research by all three scientists contributed to the scientific underpinning for the Intergovernmental Panel on Climate Change's 1996 conclusion regarding a "discernible human influence" in climate change.

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SC-Funding Office: Office of Biological and Environmental Research

6.29 Listening to the Ocean's Temperature

The 1998 North Pacific Acoustic Laboratory cruise (NPAL '98) aboard Scripp's R/V Melville involved deployment of instrument arrays essential to the Acoustic Thermometry of Ocean Climate (ATOC) experiment.

Map of a feasibility study of acoustic thermometry in the North Pacific Ocean. Lines represent acoustic paths from sound sources on the U.S. West Coast and in Hawaii to U.S. Navy and other receivers. Paths cover distances of up to 3,100 miles (5,000 km) in the North Pacific, with a 6,200 mile (10,000 km) path to New Zealand. ATOC represents the first attempt to directly provide average measures of temperature throughout much of the Pacific Ocean basin.

Acoustic thermometry is a method that was devised for tracking long-term changes in ocean temperature by using low-frequency sounds transmitted across ocean basins at a particular depth. The technique, which works because the speed of sound is proportional to water temperature, was invented by Walter Monk at Scripps Institute of Oceanography and Carl Wunsch at Massachusetts Institute of Technology, with support from the Office of Science. It turns out that acoustic thermometry is a sensitive technique not only for measuring the average temperature of vast expanses of ocean but also for tracking long-term changes in ocean climate associated with global warming. The idea works by sending sound signals from underwater speakers and tracking how long it takes them to reach receivers moored to the ocean floor thousands of miles away. Because sound travels faster in warmer water; slower in cooler water, recording increasingly faster travel times of the sound waves would indicate the ocean is warming. The concept was proven about 10 years ago, when the Office of Science and several other agencies demonstrated that acoustic thermometry could generate high-fidelity global and basin scale ocean thermal data.

Scientific Impact: Acoustic thermometry is more sensitive than local measurements for tracking long-term trends in ocean temperature because it can detect changes in deep ocean areas that exhibit little, if any, seasonal or interannual variation. This technique reduces the time required to detect a trend in climate warming from several decades to as little as a decade.

Social Impact: Acoustic thermometry helps to improve the science base for societal decisions and policymaking with regard to human activities that contribute to global warming. It may also reveal information about other oceanographic phenomena, such as El Nino events, that have profound effects on climate.

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SC-Funding Office: Office of Biological and Environmental Research