The Office of Basic Energy Sciences

Impacts of Basic Research

Office of Energy Research
U.S. Department of Energy

Fundamental Research and its Relevance to Energy Technologies

The Office of Basic Energy Sciences. The Basic Energy Sciences (BES) program within the U.S. Department of Energy's Office of Energy Research is one of the Nation's foremost sponsors of fundamental research in materials sciences, chemical sciences, geosciences, plant and microbial sciences, and engineering sciences. The program funds more than 2,400 researchers at 200 institutions nationwide and supports 17 major national user facilities. The BES program underpins the DOE missions in energy and the environment, advances energy-related basic science on a broad front, and provides premier national user facilities for researchers from academia, industry, and government laboratories.

BES is truly prototypical of a large, diverse, and robust fundamental research program that exists within a mission agency. To fulfill its mission -- *"to foster and support fundamental research in the natural sciences and engineering leading to new and improved energy technologies and to the understanding and mitigation of the environmental impacts of energy technologies"* -- the BES program strives to at once achieve excellence in basic research; relevance to a broad national energy agenda; and stewardship of human resources, essential scientific disciplines, institutions, and premier user facilities.

Making Basic Research Relevant. To bring about research relevance, BES sets strategic research directions through working relationships with other DOE programs; through research workshops involving input from the scientific and technical communities; through the promotion of open information transfer and exchange of ideas between the basic and applied research communities; and, finally, through the sponsorship of selected high-impact research collaborations and partnerships. Individual research projects are funded based on peer review by the members of the scientific community. These approaches to basic research funding have led to 120 Cooperative Research and Development Agreements (CRADAs), which extend the basic research to applications and development. In addition, there are literally hundreds of collaborations between BES researchers and industrial researchers.

The resulting diverse portfolio of basic research programs and the combination of university and laboratory programs enables interdisciplinary research needed to solve the problems of energy production and use and also integrates basic science with applied science and development activities. The Department's national laboratory system plays a special role in the ability of BES to effectively integrate research and development by providing opportunities to collocate activities at these sites. For example, about one third of scientists supported by BES at the national laboratories also receive support from at least one of DOE's technology programs. In this way, BES helps guarantee that energy technology development is being conducted with benefit from advanced scientific knowledge and that the basic research programs are focused in areas directly relevant to energy systems.

The Impact of Basic Research on Energy Technologies. BES research activities impact DOE's energy missions in Energy Resources, National Security, and Environmental Quality. The information on the following pages focuses on the relevance of BES research to the Energy Resources missions of the Department and does not include similar examples for National Security and Environmental Quality. The summary table on the next page shows that the areas of fundamental research supported by BES are integrated to energy technologies both through linkages with the applied research and development activities supported by DOE Energy Resources programs and through direct collaboration with U.S. industry. The 17 BES research areas described on the subsequent pages and their success stories illustrate how new knowledge gained through basic scientific research is quite often applicable to a number of different energy technologies.

The FY 1997 funding level and the number of projects at universities, laboratories and industry supported by BES for each research area are given at the bottom of each vignette. A summary of each BES project can be found by using the key-word index references provided for the five BES Annual Summary Books. The Annual Summary Books can be obtained by calling the BES office at (301) 903-3081 or through links on the BES homepage

(http://www.er.doe.gov/production/bes/).

Examples of Fundamental Research Programs in the Office of Basic Energy Sciences (BES) and their Relevance to Energy Technologies (excludes National Security and Environmental Quality)

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. industry

	Transportation Technologies		Seven* Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
	EE / OTT	Industry	EE / OIT	Industry	EE / OUT	Industry	EE / BTS	Industry	FE	Industry	NE	Industry	ER / FES	Industry
Advanced Battery Research	X	X												
Advanced Separations and Actinide Science			X	X	X					X	X	X		
Catalysis Research			X	X					X	X				
Ceramic Science	X	X	X						X	X			X	
Combustion Related Research	X	X	X	X	X	X		X	X	X				
Corrosion Science		X		X		X			X	X		X		
Geochemistry of Fluid-Rock Interactions					X	X			X	X		X		
Intermetallics Science			X	X					X	X				
Microbial Fuel Conversion	X		X		X	X								
Nonlinear Fluid and Gas Dynamics		X		X		X			X	X		X		
Photovoltaics and Semiconductors	X	X			X	X	X	X	X	X	X		X	
Plant Energy Conversion	X			X	X	X								
Radiation Materials Science					X				X		X	X	X	X
Rock Mechanics, Fracture, and Flow					X	X			X	X		X		
Solar Photochemical Energy Conversion				X	X		X							
Superconductivity					X	X			X				X	
Welding and Joining Science	X	X	X	X		X			X	X				

* The seven industries that consume 80% of the energy and produce over 90% of the wastes in the manufacturing sector are: steel, aluminum, forest products, glass, metalcasting, chemical, and petroleum refining.

Department of Energy (DOE) Organizational Symbols:

Programs areas included among these examples:

EE, Office of Energy Efficiency and Renewable Energy
- OTT, Office of Transportation Technologies
- OIT, Office of Industrial Technologies
- OUT, Office of Utility Technologies
- BTS, Office of Building Technology, State, and Community Programs

FE, Office of Fossil Energy
NE, Office of Nuclear Energy, Science and Technology
ER, Office of Energy Research
- BES, Office of Basic Energy Sciences
- FES, Office of Fusion Energy Sciences

Programs areas NOT included among these examples:

National Security Programs
- DP, Office of Defense Programs
- NN, Office of Nonproliferation and National Security

Environmental Quality Programs
- EM, Office of Environmental Restoration and Waste Management
- RW, Office of Civilian Radioactive Waste Management
- EH, Office of Environment, Safety and Health

ADVANCED BATTERY RESEARCH

The Office of Basic Energy Sciences (BES) Advanced Battery Research program supports fundamental research in areas critical to understanding the underlying limitations in the performance of non-automotive electrochemical energy storage systems. Areas of research include the characterization of anode, cathode, and electrolyte systems and their interactions. The program covers a broad spectrum of research including fundamental studies of composite electrode structures, failure and degradation of active electrode materials, and thin film electrodes, electrolytes, and interfaces. The aim is providing knowledge that will lead to improvements in battery size, weight, life, and recharge cycles.

Coordination of these basic research efforts with applied research programs is accomplished government-wide by participation in the Interagency Power Working Group. Close coordination with the Exploratory Battery Program in the Office of Energy Efficiency and Renewable Energy's Office of Transportation Technologies (EE/OTT) is accomplished through joint program meetings, program reviews, and strategy sessions. Additional coordination with industry users and their customers is accomplished through participation in the National Electronic Manufacturing Initiative.

SUCCESS STORIES

Non-aqueous Electrolytes. Fundamental research in the deposition of reactive metals and their mobility and stability in non-aqueous electrolytes at Lawrence Berkeley National Laboratory by Charles Tobias with support from BES's predecessor organization in the early 1960's identified those organic electrolytes that led to the development of the current generation of high energy and power lithium and lithium ion batteries. Because of their performance advantages, they are now widely used in consumer and defense applications and are under further development for use in electric vehicles by EE/OTT.

New Solid Polymer Electrolyte. Collaborative research between Khan and Fedkwi at North Carolina State University and Baker at Michigan State University has resulted in a new solid polymer electrolyte system that exhibits high room temperature conductivity. This advance resulted from the ability to minimize the strength of the interaction between the lithium complex and the polymer network by controlling the void volume of the network and the hydrophobicity of the interface. The potential impact of this discovery on battery technology is in a critical problem area for achievement of the U.S. Advanced Battery Consortium goals. The research has resulted in a partnership between BES and the EE/OTT for continued exploration of the underlying science and rapid transition of research results to practical applications.

Thin Film Rechargeable Battery. Fundamental research in ion transport in glassy solids at Oak Ridge National Laboratory has led to the successful development of thin film lithium battery technology that has produced batteries half the thickness of household saran wrap. The thin film battery technology was aided by EE/OTT applied research funding and has resulted in four CRADAs and one commercial license for applications in medical, electronics, and telecommunications devices.

Rechargeable Battery Technology Cooperatively Transferred. Basic research in non-aqueous liquid electrolyte systems has led to an approach for prevention of the oxidation of alkali metal electrodes by the electrolyte. The same chemistry that is operable in flame retardants, such as Halons, is applicable to the redox chemistry in alkali metal batteries. The research carried out at the Stanford Research Institute by Smedley has led to the development of a non-flammable organic liquid electrolyte for lithium and lithium ion battery systems. The modified electrolyte has improved the safety of rechargeable batteries. The technology has been further developed by the CIA Office of Research and Development for use in a government manufacturing process.

BES FY 1997 Funding: $4.3 M
Number of BES Projects: 31 (15 Laboratories; 16 Universities)

Program summary book index reference:
FY 1996 Chemical Sciences: Advanced Battery Research

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X	X												

ADVANCED SEPARATIONS AND ACTINIDE SCIENCE

Separations processes constitute a significant component of the cost of most raw materials and are of great importance to the cleanup of wastes at Department of Energy (DOE) sites. Current processes are energy intensive, lack specificity, and could be improved by the development of models to enable the design of approaches for specific separations problems. Basic Energy Sciences (BES) research seeks to improve our understanding of chemical and physical properties that are fundamental to separations. Research in actinide chemistry elucidates the chemical and physical properties of actinide elements. The molecular level understanding that stems from BES programs provides a basis for the development of advanced processes for the production, use, safe handling, storage, and disposal of actinides and their fission products. Programs in separations and actinide research are highly integrated by virtue of extensive collaborations and close cooperation between researchers, which has a long and successful history.

SUCCESS STORIES

Inorganic Membranes Show Reverse Molecular Weight Selectivity for Hydrocarbons. Efficient utilization and transport of natural gas requires the separation of light hydrocarbons to adjust the heating value of the natural gas to pipeline specifications. One of the by-products of this separation is the heavier high value natural gas liquids (NGLs). Processes currently in use require energy intensive cryogenic distillation, the high costs of which are offset by the value of NGLs as petrochemical feedstocks. Better economics and energy savings could be obtained with membranes if their size discriminating selectivity could be reversed. The desire for reverse selectivity membranes arises from the need to recompress the natural gas after separation, a very costly process. Reverse selectivity membranes would provide the high pressure pipeline quality natural gas and the high value NGLs without cryogenic distillation. Fundamental studies of the transport mechanisms in inorganic membranes, performed by J. D. Way and coworkers of the Colorado School of Mines, have led to the development of a "reverse selectivity" membrane which, remarkably, transports heavier hydrocarbons faster than lighter ones. The key to reversing the selectivity was the creation of an environment where chemically selective transport mechanisms dominate those based on size discrimination. These new membranes could be commercially important because of their potential to form the basis for new or modified processes that bypass the energy-intensive and costly recompression step.

"Green" Separation Process for Hanford Wastes Emerges from Fundamental Studies of Crown Ethers. The radioactive components in the Hanford waste tanks comprise a mere 1/100th of a percent of the millions of gallons of contaminated waste in storage. Highly selective removal of the radioactive components could significantly reduce the volume of waste which would otherwise require very costly processing and long-term storage. BES-supported fundamental studies of technetium extraction, conducted by Bruce Moyer and co-workers at Oak Ridge National Laboratory in the 1980s, followed by more recent investigations of the structural and thermodynamic aspects of the extraction of alkali metal salts with crown ethers has led to a new technetium extraction process. The crown ether binds sodium ions already present in the waste and then extracts technetium as much as four orders of magnitude better than other ions, some of which are present at much higher concentrations. The crown ether complex is readily decomposed by contact with water to release the extracted technetium, thereby affording a convenient, safe, and economical stripping method. The crown ether is then recycled thus minimizing secondary waste production. Support from BES provided fundamental science that led to the development of this new waste remediation technology under the Efficient Separations and Processing Crosscutting Program of the Office of Science and Technology in the Office of Environmental Management.

Enhanced Separation of Heavy Elements. Research on actinide separations at Argonne National Laboratory has had a long, successful history impacting nuclear technology. Beginning with the discovery of the extractant CMPO (carbamoylmethyl phosphine oxide) in 1981, the research led to the development of a new solvent extraction process in 1985 that became known as TRUEX. The TRUEX process allows the extraction of all actinides from a nitric acid medium. This process became significant in purification and reprocessing of nuclear fuel. Recently, this initial discovery together with continued research on separation systems and new complexants, has led to the development of DiPhonix7 Ion Exchange Resins. These resins are used for the removal of radioactive and hazardous metal ions from aqueous solutions and organic solvents. This development led to an R&D 100 Award in 1994 and provided the foundation for formation of a new company, Eichrom, Inc., in Chicago. The company has been highly successful in marketing the resins for the treatment of low level radioactive waste from nuclear power plants and for iron control in hydrometallurgical processing of copper. The initial discovery of CMPO and other investigations into waste treatment also provided the foundation for the yttrium-90 separation process highlighted below.

Nuclear Waste Used in Cancer Treatment. A process for the removal of strontium-90 from nuclear waste has been adapted to the preparation of yttrium-90 in high yield and with the purity required for targeted cancer treatment. An extraordinary separation factor of greater than 10^9 for yttrium was achieved, thus producing yttrium-90 with zirconium levels that offer no interference with bonding of the radioactive yttrium-90 to monoclonal antibodies. The process uses only nitric acid and water as reagents, making it simple and inexpensive. The fundamental research basic to the development of the separations processes was supported by BES at Argonne National laboratory; the Office of Nuclear Energy supported the isotope production and distribution activities at Pacific Northwest National Laboratory.

BES FY 1997 Funding: $8.3 M
Number of BES Projects: 28 (15 Laboratories; 13 Universities)

Program summary book index reference:
FY 1996 Chemical Sciences Division: Actinide Chemistry and Separations, sub-heading Extractions

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
		X	X	X					X	X	X		

CATALYSIS RESEARCH

Catalysis is a chemical process found widely in nature and used extensively in industry because it removes energy barriers to chemical reactions. Catalysts used for the refining of petroleum or the manufacture of chemicals are important because they reduce process energy, speed up production, and make possible the manufacture of new materials. Despite their importance, catalytic processes are not sufficiently well understood to allow for rational design of new catalysts. Models for catalytic action are limited in scope and applicability. The Office of Basic Energy Sciences (BES) catalysis program seeks to gain understanding of catalysis at the molecular level to allow the development of general theories and models of catalytic action. The program includes both heterogeneous (multiple phases such as liquid/solid) and homogeneous (single phase) catalysis. Research in heterogeneous catalysis seeks to characterize the role of surface properties on molecular transformations and the structural relationships between oxide surfaces and reaction pathways, especially in the acid and redox catalysts commonly encountered in industrial applications. Research in homogeneous catalysis seeks to characterize the activation and subsequent reactions of carbon-hydrogen bonds and the role of bonding and molecular structure on the catalytic processes. The program constitutes the largest single component of the Nation=s basic research portfolio focused on chemical catalysis.

Coordination activities have included Office of Energy Efficiency and Renewable Energy (EE), the Office of Fossil Energy (FE), and the National Science Foundation, academic researchers and industry=s involvement in developing the ACatalysis Roadmap to the Future@ which serves to clarify the catalysis contribution to AThe U.S. Chemical Industry - Technology Vision 2020@ document.

<u>SUCCESS STORIES</u>

<u>New Metallocene Catalysts Lead to Commercial Applications</u>. Research at Northwestern University led by Tobin Marks and at California Institute of Technology led by John Bercaw have substantially contributed to the development of a new class of metallocene polymerization catalysts in which polymerization occurs at a highly specific metal site within a well-defined coordination environment. Owing to the stereospecific nature of their action, the homogeneous metallocene systems represent a substantial advance over the prior heterogeneous polymerization catalysts. Recent advances on two fronts, strained early transition metals (Cal Tech) and non-coordinating counterions (Northwestern), have resulted in new commercial applications by Dow Chemical and by Exxon Chemical. The remarkable stereospecificity features of these new catalysts have not only led to a variety of new, advanced polymer products over a wide range of densities but also provide the ability to understand in detail the underlying molecular mechanisms, thus allowing rapid design of improved catalysts for specific products. The new polymers produced from these catalysts are found in wide-ranging applications from food wrapping to the plastic front end front bumper combinations on automobiles. The impact of these new products can be envisioned from the Dow Insite process, which produces plastics with a market value of about $2B per year at Dow=s Texas plant.

<u>New Graphite Nanofibers Store Hydrogen</u>. Basic research can often lead to unexpected applications. A new nano-phase graphitic material capable of absorbing as much as three grams of hydrogen for each gram of carbon has been discovered by researchers studying catalyst deactivation. The origins of this material are found in studies of metal particle fracturing that occurs during catalysis. In the course of her investigations on the role of carbon fibers in fracturing metal particles, Professor Nelly Rodriguez of Northeastern University found that the graphitic microstructure of the fibers was such as to allow hydrogen to fit within the interplanar space between aligned graphitic planes. Based on the insight developed from these studies, Professor Rodriguez developed the synthetic routes to these new nanomaterials in an independent research effort, for which she has recently been awarded a patent. Although it is not yet understood how these nanofibers absorb such a large volume of hydrogen (about 32 liters of hydrogen per gram at room temperature and elevated pressure), the discovery is potentially very significant to hydrogen storage technology, and perhaps also to storage of other small gases. Further development of this nanofiber technology has recently been funded by the Office of Energy Efficiency.

<u>Fundamental Studies on Metal-catalyzed Polymerizations Lead to Current and Near-term New Materials Applications</u>. Two recent reports from *Chemical & Engineering News* furnish compelling evidence of the long term benefits of BES funded research. The May 5, 1997, issue reports Shell Chemical=s recently announced plans to build a 55 million-lb-per-year aliphatic polyketone polymers plant at their site in Geismar, LA. Professor Ayusman Sen (Pennsylvania State University) points out that the palladium-based catalytic system used by Shell in this process is derived from his BES-funded work. Shell initiated work following the Sen group=s initial publications in 1982, with the first patent

being issued in 1984. Current uses for these polyketone polymers include gears for business machines, liners for flexible fuel hoses, and industrial molded parts. The second report (April 5, 1997, issue) highlights the Sen group=s recent discovery of a low-cost, catalytic route for the manufacture of advanced polymer materials, namely, polyoxalate polymer resins, now under study for use in making bioabsorbable sutures. Current methods used to make polyoxalates require costly oxalic acid, or similarly expensive starting material. Sen=s group has discovered a catalytic method to prepare the polyoxalate resins from less expensive alkylene dinitrites and carbon monoxide.

BES FY 1997 Funding: $21.7 M
Number of BES Projects: 138 (37 Laboratories; 101 Universities)

Program summary book index reference:
FY 1996 Chemical Sciences: Catalysis and Surface and Interface Chemistry
FY 1996 Materials Sciences: Phenomena, sub-heading: ACatalysis@

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
			X	X				X	X				

CERAMIC SCIENCE

Ceramic materials play an integral role in the utility, automotive, and other energy-intensive industries. A fundamental understanding of their complex microstructure and behavior is essential for their successful implementation. The Ceramic Sciences program addresses the scientific issues underlying the synthesis, processing, behavior, and characterization of ceramic and non-metallic glassy materials, which are relevant to the energy or environmental missions of the Department of Energy. Focus areas include synthesis, processing, reactivity, and physical and mechanical properties, with emphasis on elevated temperature behavior. The technological areas impacted include high temperature structural materials (e.g., high temperature monolithic and composite ceramics and ceramic coatings), energy storage materials (e.g., solid electrolytes, batteries, ultracapacitors) energy conversion materials (e.g., fuel cells), hazardous waste storage materials (glasses and ceramics), sensors, and environmentally benign synthesis techniques.

Integration activities occur through the Energy Materials Coordinating Committee (EMaCC), the EMaCC subcommittee on structural ceramics, the MatTec Communications Group on Structural Ceramics, and the Center of Excellence in Synthesis and Processing (CSP) projects on Materials Joining and Mechanically Reliable Surface Oxides for High-Temperature Corrosion Resistance. At the bench level there is significant co-siting of research and co-funding of principal investigators between the Office of Basic Energy Sciences (BES) programs and those of the Office of Energy Efficiency and Renewable Energy (EE), the Office of Fossil Energy (FE), the Office of Environment Management, and the Office of Defense Programs (DP).

SUCCESS STORIES

Functionally Gradient Materials Successfully Modeled. In a joint FE-BES effort, finite element models developed by B. Rabin and co-workers at Idaho National Engineering and Environmental Laboratory for the development of residual stresses in functionally graded (ceramic-metal) materials have been verified at Oak Ridge National Laboratory using high resolution neutron diffraction permitting the design of more reliable joints between ceramics and metals.

Major Improvement in the Toughness of Silicon Carbide Ceramics. A three fold improvement in fracture toughness of silicon carbide ceramics has been achieved (to ~9 MPa $m^{1/2}$) by the DeJonghe research group at Lawrence Berkeley National Laboratory. This enhancement of fracture toughness was also found at high temperatures where these ceramics would be used as a structural material for energy generation. Although silicon carbide ceramics are very strong, they are also very brittle. Hence improvement in the toughness of silicon carbide ceramics has been a long sought goal of many laboratories. Building upon an understanding of how particles in a ceramic bond together when processed at high temperatures, a process was developed that enabled grains of the ceramic to grow into interlocking plate-like grains during the bonding process. This interlocked structure greatly resists the growth of a crack, thereby increasing the fracture toughness and thus the fracture resistance of the silicon carbide.

Breakthrough in Processing of Aerogel Films. A breakthrough in the processing of ceramic aerogel films by the Brinker and Hurd group at Sandia National Laboratories-New Mexico won a prestigious award of the American Chemical Society and was cited as an important discovery by the *Wall Street Journal*. This breakthrough overcame the sixty year barrier to the large scale commercial utilization of these films. Aerogel films have a foam-like structure, exceptional lightness, and transparency. They are ideal insulating materials for double-paned windows and other uses. When freshly formed from a liquid and until it hardens, the film can be easily torn. Older processes required a toxic liquid and high pressure and temperature to dry the films. Employing a new understanding of film drying and chemical treatment of the surfaces of the pores in the film, a non-toxic, low-pressure and temperature process was developed to keep the film flexible and resilient as it hardened.

New Process to Form Diamond-Like Boron Nitride Films. A process to grow diamond-like boron nitride films, the second hardest known material, has been discovered by the McCarty group at Sandia National Laboratories-California based on a new understanding of how hard nitride films are formed. Since boron nitride (unlike diamond) does not react with iron or steel, it is an ideal material for cutting tools. Films of boron nitride (like diamond) can be grown from hot gases and plasmas without the use of high pressures. However, it was discovered that to grow films of boron nitride which contain the hard, diamond-like form rather than the soft graphite-like form requires irradiation of the film with a low-energy beam of ions. This new process to form ultra-hard boron nitride films could revolutionize the cutting tool industry.

Fundamental Studies of Colloid Surface Chemistry Advance Studies of Radioactive Tank Waste Processing. Two key discoveries by the Bunker group at Pacific Northwest National Laboratory highlight the importance of fundamental studies in understanding the behavior of tank wastes and their eventual processing. First, transmission electron microscopy demonstrated that tank wastes consist predominately of extremely small (sub-micron) particles of insoluble oxides, hydroxides, and salts. The second key of the discovery was the realization that the physical properties of the wastes are controlled by agglomeration of the sub-micron particles. The types of agglomerates that form are critically dependent on the surface chemistry and interaction potential between the various particles in the system. Since classical electrical double-layer theory does not apply in the high-salt content, high-pH regime of tank wastes, significant efforts are now underway to obtain the properties data necessary to further extend current models to adequately describe the range of waste properties.

Toughened Silicon Nitride Ceramics Also Require Interface Debonding for Maximum Toughness. Like many other ceramics the use of elongated grains or the addition of whiskers are used to improve the toughness of silicon nitride and Si-Al-O-N ceramics. The improved properties result when a crack causes interfacial debonding between the toughening component and the matrix, forcing the crack to follow the contour of the component rather than allowing it to take the shortest path. Researchers in the Becher group at Oak Ridge National Laboratory found that optimum debonding requires close control of yttria additions, the composition of a glassy phase used to coat the toughening component or of the Si-Al-O-N glass to maximize the toughness of ceramic.

Commercialization of Gelcasting. Gelcasting, a forming process similar to slip casting for molding of near-net shape ceramic parts, was initially developed at Oak Ridge National Laboratory under a program funded by EE. Due to low solids loading of the gels, it proved difficult to commercialize until BES powder processing expertise, also under the Becher group at Oak Ridge National Laboratory, was teamed with the EE development team and their expertise was brought to Allied Signal through the National Institute of Standards and Technology Advanced Technology Program. Allied Signal subsequently licenced this technology for commercial production.

BES FY 1997 Funding: $ 31.5 million
Number of BES Projects: 107 (63 Laboratories, 43 Universities, 1 Industry)

Program summary book index reference:
FY 1996 Materials Sciences:
MATERIALS: Amorphous State: Non-Metallic Glasses (other than Silicates); Amorphous State: Non-Metallic Glasses (Silicates); Carbides; Carbon and Graphite, Composite Materials--Structural; Dielectrics; Fast Ion Conductors; Glasses; Ionic Compounds; Nitrides; Oxides: Binary; Oxides: Non-Binary, Crystalline; Radioactive Waste Storage Materials; Solid Electrolytes; Structural Ceramics

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		ission Energy echnologies		usion Energy echnologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X	X	X						X	X			X	

COMBUSTION RELATED RESEARCH

Basic research in combustion, as supported by the Office of Basic Energy Sciences (BES), provides knowledge on the rates and energetics of chemical reactions and on the interactions of fluid dynamics and chemistry. This knowledge is required by combustion models used for the design and optimization of energy-efficient, reduced-emission combustion devices. Knowledge gained consists of measured properties as well as theoretical constructs for the reliable prediction or extrapolation of such properties. BES also supports the operation of the Combustion Research Facility (CRF) at Sandia National Laboratories, California, where collocated research, supported by BES, the Office of Energy Efficiency and Renewable Energy (EE), the Office of Fossil Energy (FE), and industry, is conducted in a highly collaborative environment. The CRF, in addition to its research contributions, serves as the focus for the integration of BES basic combustion research with the applied programs of the department and with research programs in other Department of Energy laboratories. In addition, coordination within DOE funding offices is carried out by the Combustion Coordinating Committee, with representatives from BES, EE and FE.

SUCCESS STORIES

A New Marker for Combustion. The simple radical HC, consisting of a hydrogen atom and a carbon atom, has been long believed to be a significant indicator of flame heat release. The HC spectral signature is widely used as a combustion diagnostic in applications ranging from diesel engines through industrial combustors to processes for forming diamond surfaces. In a novel, elegant experiment recently conducted at the CRF by Phillip Paul, the significance of the HC radical as a flame diagnostic has been shown to be overestimated. Rather the HCO radical, which contains an additional atom of oxygen, is indicated to be the better marker for identifying flame fronts and for measuring local flame heat release rate. As a result of this research, reliable techniques to measure HCO radicals in flames are being pursued and the standard model for the mechanism of methane combustion proposed by the Gas Research Institute is being re-examined.

Combustion Research for Industrial Processes. A four year program involving DOE, EPA, universities, and a number of industry partners in the Petroleum Environmental Research Forum came to a successful conclusion in FY 1997. The program was designed to provide the knowledge needed to formulate sensible, cost-effective air toxics regulations for process heaters and industrial boilers mandated by the 1990 amendments to the Clean Air Act. Central to this program was the Burner Engineering Research Laboratory at the CRF whose construction was a joint project between BES, the EE Office of Industrial Technologies, and the Gas Research Institute. In the invitation to the close-out briefing, James Seabold, representing the industrial partners, described the program as having been Asuccess beyond our dreams and we are, at this moment, bringing the strength of new knowledge and fundamental understanding to the Industrial Combustion Coordinated Rulemaking process.@

Diesel Collaboratory. In a collaboration involving the EE Office of Transportation Technologies and BES, building on a successful CRADA between Sandia National Laboratories, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and three major diesel engine manufacturers, and with additional support from the ER Office of Computational and Technology Research, a major program has evolved for the development and validation of combustion models in heavy duty diesel engines to guide soot elimination strategies. The CRF serves as the focus of this effort and the advanced computational and communication technologies that will be employed will allow the industry, university, and DOE laboratory partners to work together with enhanced efficiency. The work under this CRADA has already demonstrated that the previously accepted model for soot formation in diesel engines was incorrect, and the new knowledge will influence future engine design.

BES FY 1997 Funding: $11.4 M
Number of BES Projects: 64 (12 Laboratories, 52 Universities)

Program summary book index reference:
FY 1996 Chemical Sciences: Combustion

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X	X	X	X	X	X		X	X	X				

CORROSION SCIENCE

The importance of the scientific understanding of corrosion is emphasized by the estimate that corrosion in the U.S. has an economic cost of 4 percent of the gross domestic product. Corrosion damage limits the performance of all energy conversion technologies. The Office of Basic Energy Sciences (BES) basic research underlying the science of corrosion focuses on the formation, properties, and breakdown of passivating films; on a wide array of electrochemical phenomena involved in aqueous corrosion such as pitting and crevice corrosion; on high-temperature gaseous corrosion; and on new techniques to identify and study corrosion.

BES research is collocated with the Office of Energy Efficiency and Renewable Energy (EE) and the Office of Fossil Energy (FE) application and development efforts at DOE national laboratories. BES, through its Center of Excellence for Synthesis and Processing of Advanced Materials, supports jointly with EE and the Electric Power Research Institute (EPRI) a five laboratory collaboration entitled AMechanically Reliable Surface Oxides for High-Temperature Corrosion Resistance.@ For the past 20 years, researchers from both universities and the national laboratories have met regularly with researchers from EPRI and industrial laboratories at the Corrosion Contractors Meeting to exchange views and research results.

SUCCESS STORIES

Solving Problems in Power Plant Chemistry. Fundamental research at the Oak Ridge National Laboratory on high-temperature aqueous chemistry contributes to the world-wide basis for the nuclear and the fossil power industries' process controls. For example, computer codes employed by chemists at General Electric, Westinghouse, Babcock and Wilcox, Combustion Engineering, as well as the (EPRI), and the major utilities, extensively employ the chemical properties database generated by the Oak Ridge National Laboratory program to address issues of corrosion, deposition, and process control for steam generators, steam turbines, and primary circuit chemistry. Chemical properties of important additives such as volatile and nonvolatile buffers of acidity, neutron poisons, and corrosion inhibitors; contaminants such as corrosion products, chlorides, and sulfates; and even of water itself have been determined definitively with unique experimental facilities developed over many years with BES support.

X-Rays Aid the Study of Corrosion in Microchip Processing. Scientists at Brookhaven National Laboratory and IBM=s T. J. Watson Center are using x-rays from Brookhaven=s National Synchrotron Light Source to understand and mitigate corrosion during the production of integrated circuits used in computers and other electronic products. The constituent elements of a material absorb x-rays at characteristic wavelengths of x-radiation. This absorption can be used to identify which elements are present by x-ray absorption spectroscopy. The researchers applied this principle to the study of thin films that can function as conductors in integrated circuits. Their work led to an understanding of how phosphorus resists corrosion in copper anodes, used in electroplating the circuits. The collaboration has also developed a new technique for studying rapid oxidation in thin metal films. This method is now being developed for proprietary microelectronics research at IBM.

A New Tool for Use in Finding Nontoxic Corrosion Inhibitors. In collaborative work with W.R. Grace & Co., chemists at Brookhaven National Laboratory are testing nontoxic, environmentally acceptable chemicals that prevent corrosion. They are using a special Avibration probe@ in a chemical technique developed at Brookhaven. In this technique, a vibrating sensor monitors the current in an electrochemical cell. The sensor can distinguish current changes over a distance as small as 100 micrometers. The vibration probe offered a quick way to test nontoxic corrosion inhibitors developed at W.R. Grace. The investigation led to the development of effective new mixtures of inhibitors without chromates, heavy metals or phosphates.

BES FY 1997 Funding: $5.4 million
Number of BES Projects: 42 (29 Laboratories, 13 Universities)

Program Summary Book index reference:
FY 1996 Materials Sciences: corrosion: aqueous; corrosion: gaseous; corrosion: molten salt; stress-corrosion

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
	X		X		X			X	X		X		

GEOCHEMISTRY of FLUID-ROCK INTERACTIONS

The Office of Basic Energy Sciences (BES) Geosciences Research Program supports geochemical research in rock-fluid interactions to provide fundamental information on the governing mechanisms and rates of reactive geochemical processes that concentrate, transport, modify, and emplace energy resources and the by-products of energy use within the Earth's shallow crust. This basic information is significant for current and future energy technologies, particularly geothermal energy and oil and gas, as well as for understanding the disposition of wastes generated by the technological enterprise, including the by-products of nuclear energy. The BES research at the DOE national laboratories is collocated with the Office of Energy Efficiency and Renewable Energy (EE), the Office of Fossil Energy (FE), and the Office of Environmental Management (EM) supported application and development projects. Collaborative projects are common among researchers from National Laboratories, universities, and industry. Additional integration takes place through joint participation in workshops on research results and outstanding research needs.

<u>SUCCESS STORIES</u>

<u>Geochemistry of Oil and Gas Reservoirs: Oil and Gas as Renewable Resources</u>. Basic Energy Sciences-supported researcher Jean Whelan is investigating possible replenishing of oil reservoirs in Eugene Island Block 330 in the Gulf of Mexico. The research by Dr. Whelan, of the Woods Hole Oceanographic Institute, has provided geochemical evidence in support of the hypothesis that the reservoirs at Eugene Island are being replenished by recent episodic injections of gas-charged hydrocarbons from depth. The possibility, although still controversial, that replenishment is occurring in Gulf Coast and other producing areas is significant for estimating the Nation's oil and gas reserves. The geochemical research at Woods Hole is a portion of a larger university/industry consortium of researchers identified as the "Global Basins Research Network" and takes advantage of samples made available through drilling programs and research supported by industry and FE.

<u>High-Resolution X-ray Imaging of Trace Metal Distribution in Geologic Samples</u>. The first experiments on natural samples were conducted with the newly constructed beamline for geosciences/soil/environmental GeoSECARS research at the third-generation synchrotron x-ray source at the Advanced Photon Source, Argonne National Laboratory. This research provides direct molecular-scale information on local structural and chemical changes that govern mechanisms of mineral-fluid interactions. The first x-ray absorption spectroscopy experiments, in April-May, 1997, provide images at the micron-scale of the distribution of trace metals and the oxidation state of Se in the vicinity of an organism known to concentrate this element, in reduced state, from groundwater contaminated with more toxic mobile, oxidized Se-bearing species. These experiments take advantage of the extremely high brilliance and specially designed microfocusing mirrors to provide images of the micro-variability in distribution and speciation of trace elements under conditions appropriate for near-surface environments. Additionally, these advances make it possible to obtain molecular-scale information at the interface between chemically complex, physically heterogeneous mineral samples and reactive aqueous fluids, which governs the uptake and release of toxic metals significant for issues concerning the disposition of technological waste.

<u>BES FY 1997 Funding</u>: $5.8 million
<u>Number of BES Projects</u>: 35 (23 Universities; 12 Laboratories)

Program summary book index reference:
<u>FY 1996 Geosciences Research</u>: GEOCHEMISTRY, Rock-Fluid Interactions

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
				X	X			X	X		X		

INTERMETALLICS SCIENCE

Intermetallic compounds are metal to metal compounds with definite stoichiometry. Intermetallic alloys made from these compounds constitute a unique class of high-temperature structural materials as they possess the desired properties of high strength, oxidation and corrosion resistance, low density, and a high melting point. Such properties make them attractive as constituents for gas turbine engines, high-temperature coatings, and in dies and molds for ceramic and metallurgical processing. Intermetallic compounds may also be used in a variety of electromagnetic areas including both hard and soft magnets, superconductor, semiconductor, and optical applications. Under collaborations and joint sponsorships among the Office of Basic Energy Sciences (BES), the Office of Energy Efficiency and Renewable Energy (EE) Advanced Industrial Materials Program, and the Office of Fossil Energy (FE) Advanced Research and Technology Development Program, work is underway to understand, develop, test, and apply several intermetallic alloys in industrial settings. These programs have focused on the basic understanding of materials properties, particularly the role of boron additions and stoichiometry on mechanical and environmental behavior (BES); on alloy development and industrial testing for oxidizing environments (EE); and on alloy development for sulfidizing environments (FE). Additional work is supported in BES programs to investigate the potential of other classes of intermetallic alloys (e.g., laves phase alloys) for future development efforts.

Integration activities occur through the Energy Materials Coordinating Committee and the Center of Excellence for the Synthesis and Processing of Advanced Materials (nine laboratory coordinated project) on Ultrahigh Temperature Intermetallics. At the bench level, there is significant co-siting of research between programs, particularly at Oak Ridge National Laboratory (ORNL) and Los Alamos National Laboratory (LANL).

SUCCESS STORIES

Improving Intemetallic Alloys. Nickel aluminides have been successfully tested as transfer rolls for re-heat furnaces in steel manufacture, furnace trays, and dies for glass manufacture and the fabrication of Asuper@ magnets. Fundamental understanding of the role of boron additions in improving mechanical behavior and reducing environmental effects was supported by BES. Further alloy development and industrial testing was supported by EE.

Ductility in Ni_3Al Achieved. The utilization of intermetallics is often limited by their low ductility and brittle fracture at ambient temperatures. Exploratory research by the Liu group at ORNL discovered a method to ductilize Ni_3Al through boron additions and stoichiometry control. With further support provided by EE and FE, this achievement has led to the development of commercial Ni_3Al and Fe-modified alloys for industrial use.

Cause of FeAl Brittleness Discovered. Research by Liu and colleagues at ORNL have recently proven that embrittlement in FeAl is due to ambient moisture. Their first principles quantum mechanical calculations indicate that moisture-induced hydrogen reduces the atomic bonding strength by 70 percent. This discovery has resulted in a new approach to alloy design of FeAl for industrial use under both FE and EE programs.

Commercialization Successes. BES researchers have worked closely with U.S. industries and DOE technology programs to identify their needs and to expedite technology transfer. Since 1983, there have been at least 12 Licenses for Nickel and Iron Aluminides Technology, 16 patents, 30 invention disclosures, and 3 R&D 100 Awards. The Exomelt process developed by ORNL with EE support for the production of nickel aluminides is particularly notable having received a 1995 R&D 100 Award and has since been adopted by industry. The underlying science was supported by BES with follow-on support from FE, EE, and the Office of Energy Research technology transfer programs.

Magnets. Work at Argonne National Laboratory, Ames Laboratory, Brookhaven National Laboratory, Idaho National Engineering and Environmental Laboratory, and Oak Ridge National Laboratory on several intermetallic magnetic compounds (e.g., Sm-Co, Fe-Co, Nd-Fe-B) has furthered understanding of how to improve their processing, microstructure, and mechanical properties while also improving the magnetism. This allows reduced weight of automotive parts containing magnets.

BES FY 1997 Funding: $ 4.9 million
Number of BES Projects: 51 (34 Laboratories, 17 Universities)
Program summary book index reference:
FY 1996 Materials Sciences: MATERIALS: Intermetallic Compounds

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
		X	X					X	X				

MICROBIAL CONVERSION

The basic research program in microbial conversion focuses on examining the metabolism, biochemistry, genetics, and physiology of organisms and consortia of organisms that degrade lignin, cellulose, and/or hemicellulose into potential fuels. The fuels include ethanol, higher alcohols, and methane. While much of the activities involve anaerobic bacteria, fungi are also actively investigated. These studies form the foundation for the efficient conversion of lignocellulosics (biomass) into potential liquid and gaseous fuels, an important component of several technology programs in the Department of Energy.

Research is coordinated through the DOE BioEnergy Coordinating Committee comprised of representatives of all DOE organizations with wide-ranging research interests in various areas of biomass energy, biotechnology, and biology.

SUCCESS STORIES

Bioproduction of Methane. Microorganisms that possess the ability to produce methane (natural gas) have been studied for a number of years, since these organisms produce a renewable energy source. This research has shown that these bacteria are very unusual biochemically. Last year, the complete genome of a methane producing bacterium was sequenced and revealed new information about the unique biochemical and genetic properties of these organisms. Recently, biochemical and genetic procedures have been developed at the University of Illinois by Dr. Ralph Wolfe and colleagues and at the University of Maryland by Dr. Kevin Sowers and associates. The new procedures will permit the genes of methane-producing bacteria to be manipulated. This development will allow scientists to understand and develop the properties of these organisms and their unusual metabolism for renewable energy production.

Sugar metabolism. Studies conducted by Dr. Lonnie Ingram and colleagues at the University of Florida demonstrated that bacteria prefer certain sugars and go to considerable effort to metabolize a particular monosaccharide. Several bacteria have been shown to actively transport di- and trisaccharides into the cell, cleave out the preferred monosaccharide, and export the less preferred sugar components. The exported sugars may eventually be used for growth after the preferred monosaccharides are totally consumed. It is important to understanding how microbes select and metabolize individual monosaccharides in order to efficiently use biomass resources which contain varied sugar constituents.

Lignin Degradation. Lignin is the most abundant polymer in nature, and the white rot fungi are among the few known organisms capable of degrading lignin efficiently. Manganese peroxidases are one class of lignin-depolymerizing enzymes found among these organisms. The white rot fungus *Phanerochaete chrysosporium* can be induced to produce a family of manganese peroxidases, each showing different kinetic properties suggesting differing preferred substrates among the complex heterogeneous lignin polymers. Efforts to isolate and characterize each member of this enzyme family have proven difficult until the recent successful transformation of another fungus, *Aspergillus oryxae*, with a manganese peroxidase gene from *P. chrysosporium*. The research group led by Dr. Dan Cullen at the University of Wisconsin has demonstrated that a single recombinant family member of manganese peroxidase can be obtained from the transformed *Aspergillus* in yields comparable to the activity of the whole family of manganese peroxidase produced by *P. chrysosporium*, and will enable characterization of each particular manganese peroxidase. Industry is interested in this transformation system for enzyme production. Lignin depolymerizing enzymes offer the potential for an effective Agreen@ technology in pulp and paper production.

BES FY 1997 Funding: $3.5 million
Number of BES Projects: 36 (35 Universiies; 1 Laboratory)

Program summary book index reference:
FY 1996 Energy Biosciences*:* Lignin-Polysaccharide Breakdown, Fermentative Microbial Metabolism, One and Two Carbon Microbial Metabolism

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X		X		X	X								

NONLINEAR FLUID and GAS DYNAMICS

The Office of Basic Energy Sciences (BES) Engineering Program supports fundamental research on broad, generic topics in energy related engineering topics. This includes research on fractals and porous media transport, nonlinear waves, traveling wave convection in fluid mixtures, wave turbulence interactions, multiphase systems, gas and solids problems, the effect of different Reynolds numbers on turbulence, mixing and transport, gas-liquid flow in pipelines, lubricated transport of viscous materials, the rheology of concentrated suspensions, macrostatistical hydrodynamics, heat/mass transfer enhancement in separated and vortex flows, effect of forced and natural convection on solidification of binary mixtures, interfacial area and transfer in two-phase flow, and various diagnostics for analyzing fluids.

An emphasis of the research is on complicated fluid dynamics because fluids are a part of most energy-related systems including: pipelines, manufacturing processing, hydraulic systems, planes, trains, automobiles, ships, liquid metal handling, new materials synthesis, chaotic wave motion, weather prediction, environmental issues, and biological systems.

SUCCESS STORIES

Oil Crude Mobility Increased in Pipe Flow. Since the 1930's, engineers have attempted to flow a combination of oil crude and water unsuccessfully. A recent study using nonlinear analysis and modern high speed computers, combined with experiments in a laboratory at the University of Minnesota, has provided new models for controlling the flow. By controlling the pressure and other conditions, the water lubricates the pipe so that it is easier to pump the crude. In Canada, the Syncrude Ltd technology program was strongly influenced by these two-phase flow results. Syncrude set up a major test with a 1 km long pipe in Canada last summer. Based on the results, Syncrude is planning to install a 35 km pipe from remote oil sands to their current production site where the tar crude will be upgraded into a synthetic crude (as reported in the *Wall Street Journal*, this will be a $4.12B project). The potential economic incentives for the water-lubricated flow technology are significant compared to the alternate technologies. Syncrude is a joint venture supported in part by the U.S. firms Exxon (through Imperial Oil), Murphy Oil, and Torch.

Shell Oil Uses Our Results. The following three statements were provided by Shell Oil:

1) AA gas-condensate flowline plugged by gas hydrates can easily cost $1-3 million in lost production. Hydrate inhibitors are effective only if they continuously mix with the gas and liquid, so pipelines are designed using relations for liquid entrainment rate and droplet size developed by Professor Thomas Hanratty and his group at the University of Illinois.@
2) AFor deep water Gulf of Mexico conditions, an undersized subsea oil and gas flowline could easily cause $100,000/day in lost potential revenue. A key parameter in the design methods for pressure loss relates to the slippage between gas and liquid. The methods proposed by Andritsos and Hanratty, University of Illinois, have been shown to provide near optimum sizing relations.@
3) AOversized pipelines result in both excessive capital costs and decreased production, as low velocity fluids build up in low spots, imposing higher back pressure on the reservoir. Such an error may result in losses greater than $10 million in capital cost. Again, design methods which derive from Dukler=s work at the University of Houston as well as the work of Hanratty (Illinois) and Wallis at Dartmouth have proved essential to design.@

New catalytic control system for a lean burn engine. The Macrostatistical Hydrodynamics program funded at Los Alamos National Laboratory, Sandia National Laboratory and Massachusetts Institute of Technology developed a multiphase flow characterization and processing technology. This technology was used to develop a new catalytic control system for a lean burn engine to control the NO emissions under the Partnership for a New Generation of Vehicles (PNGV) Program. A PNGV award was given to Dr. Alan Graham of Los Alamos National Laboratory.

BES FY 1997 Funding:	$2.5 million	
Number of BES Projects:	20	(1 Laboratory; 19 Universities)

Program summary book index reference:
FY 1996 Engineering Research: Budget Number 01-C

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
	X		X		X			X	X		X		

PHOTOVOLTAICS and SEMICONDUCTORS

Research within this program area includes synthesis of new and tailored semiconductor materials; characterization of structure, electronic structure and stability of semiconductors; investigations of surfaces and interfaces; the influence of light on the behavior and properties of semiconductor materials; theory and modeling of properties and behavior; and the operation of facilities which support such research. Semiconducting materials underpin virtually the entire Ahigh tech@ industry worldwide. They comprise the building blocks and components for several technologies within the Department of Energy mission, including photovoltaics, sensors, power electronics and high speed computational systems. The Office of Basic Energy Sciences (BES) research is collocated with the Office of Energy Efficiency and Renewable Energy (EE) funded work at several national laboratories. High-Efficiency Photovoltaics is one of the thrusts under the auspices of the Center of Excellence for the Synthesis and Processing of Advanced Materials (CESYNPRO) and is jointly planned and funded by BES, EE, and Electric Power Research Institute (EPRI). Coordination is effected through the CESYNPRO and the Energy Materials Coordinating Committee, which has a Subcommittee on Semiconductors chaired by Jerry J. Smith, BES, and joint BES-EE workshops.

SUCCESS STORIES

High Efficiency Gallium Indium Phosphide-Gallium Arsenide Tandem Photovoltaic Cell. A joint BES-EE project at National Renewable Energy Laboratory has produced a tandem photovoltaic cell which holds three world records for efficiency, having achieved 29.5 percent at one sun in a flat plate cell, 30.2 percent in a 140 -180 sun concentrator cell, and 25.7 percent in a one sun space cell. The effort was begun with theoretical calculations by Dr. Alex Zunger who investigated the effect of various multilayer structures stacked on top of each other to optimize the photo conversion efficiency. These photovoltaic multilayer structures were then fabricated and tested with the remarkable results noted above. This achievement is an example of integrated research and development as practiced in a national laboratory. The fundamental investigations of the key materials science, theory and properties, were supported by BES; the cell development work has been funded by the EE Office of Photovoltaic and Wind Technologies.

Single Atom Defects in Semiconductors Observed. A technique was developed to observe single atomic defects in very small semiconductor structures, a few atomic layers thick. The presence of atomic defects in these structures can reduce the efficiency of the emission and absorption of light and the conduction of electric current. A microscopy technique was developed to image across the atomic planes of these structures. The technique enabled the chemical nature of the defects to be established and the structural and electronic ramifications of atomic defects to be determined. These observations by Eike Weber and Miquel Salmeron at Lawrence Berkeley National Laboratory provide a key insight into understanding atomic defects which degrade the performance of semiconductor structures.

Nanowires: Magic Structures and Conductance Quantization. Understanding the formation mechanisms and structural, mechanical, and electronic transport properties of wires of nanometer scale dimensions is of fundamental importance both from the scientific point of view and because of the increasing miniaturization of electronic components, mechanical devices, and machine elements. In two papers published in 1997, U. Landman and his collaborators at the Georgia Institute of Technology described results of first principles quantum simulations of atomic structure, electronic conductance, and dynamical fluctuations in metallic nanowires. The researchers discovered formation of clustered structures as the wires were stretched to a few atoms in diameter. They have predicted the spontaneous occurrence of self selecting "magic wire configurations" of enhanced stability and of unique quantized conductance properties. The results of these investigations allow deep insights into the physical nature of low dimensional materials systems and provide impetus for laboratory experiments aimed at the development of nanoscale devices and atomic scale switches.

Tenfold Increase in Electrical Conductivity of Semiconductors. Gallium arsenide is an advanced semiconductor material for electronic devices such as solar cells, diode lasers for reading compact discs, and ultra-high speed transistors. However, unless the gallium arsenide semiconductor is electrically activated, it is useless. Previous work showed that injected carbon atoms do not activate the semiconductor when injected into the gallium arsenide unless it is also injected with gallium. It was recently shown that other heavy elements can be used in place of gallium, but gallium is the most effective of the elements tested. The explanation for the increase in the conductivity is that elements such as the injected gallium create traps for the injected carbon atoms. With this new understanding, Eugene Haller of LBNL was able to achieve a tenfold increase in the number of electrical charge carriers in gallium arsenide over that obtained when only carbon is implanted.

Superconducting Silicon. A metal-insulator transition has unexpectedly appeared in a MOSFET (metal-oxide semiconductor field-effect transistor) subjected to strong electric fields at low temperatures. This is quite remarkable because a MOSFET operates as an ultrathin two- dimensional sheet of electrons on the surface of the silicon semiconductor and, according to established theory, should not conduct at very low temperatures. However, recent experiments have shown that, above a certain critical electron density, the resistivity decreases markedly by as the temperature is lowered below 1 Kelvin. The resolution of the apparent contradiction is that the electron gas is condensing into a superconducting-like state at low temperatures. That state is quenched by a magnetic field in a manner very consistent with what is observed for regular superconductors. The observations by Drs. Miriam Sarachik, Demetri Simonian, and Sergey Kravchenko have sparked considerable interest in the scientific community and were the subject of a *Search and Discovery* feature article in the July, 1997 issue of *Physics Today*.

BES FY 1997 Funding: $14.5 million
Number of BES Projects: 97 (60 Laboratories, 35 Universities, 2 Industries)

Program summary book index reference:
FY 1996 Materials Sciences: Keywords: Semiconductor Materials-Elemental, Semiconductor Materials-Multicomponent, Photovoltaic Effects.

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X	X			X	X	X	X	X	X	X		X	

PLANT ENERGY CONVERSION

Green plants and some bacteria use photosynthesis to capture solar energy and convert it into chemical energy that fuels metabolism and the biosynthesis of a broad range of storage compounds and structural components. For example, the chemical energy in firewood was the early energy source for mankind, and even today the worldwide combustion of plant biomass generates more energy than any other non-fossil fuel source. As a renewable resource, plant biomass potentially has enormously valuable uses when it is converted into specific materials, fuels, chemical feedstocks and petroleum replacing materials. Basic studies in plant biology are providing new insights into the genetic, metabolic, and enzymatic properties of plants that regulate the production of specific useful chemical compounds and materials. Similarly, studies on the regulation of the photosynthetic process that fuels metabolic biosynthesis are yielding new insights on how bacteria and plants channel photosynthetic energy into the production of renewable biomass materials.

Research is coordinated through the DOE BioEnergy Coordinating Committee comprised of representatives of all DOE organizations with wide-ranging research interests in various areas of biomass energy, biotechnology, and biology.

SUCCESS STORIES

Manipulation of Energy Resources. Cellulose is the most prevalent biological compound on earth. It is the principal component of all plants, wood, paper, and cotton. When considered globally, cellulose constitutes an enormous supply of chemical energy, all of it renewable. Recently, Dr. Chris Somerville and colleagues at the Carnegie Institution of Washington Plant Biology Laboratory have manipulated several plants to make significantly less cellulose. These altered plants are valuable because they can lead to the identification of factors that control the synthesis and deposition of cellulose and related compounds. Such knowledge may permit genetic engineering to control the way plants distribute their energy into cellulose or other chemical such as liquid fuels.

Novel Catalytic Mechanism Discovered. An enormous variety of specific chemical reactions constantly occur in live biological systems. Each reaction is precisely controlled. Enzymes are proteins that act to catalyze particular reactions such that one chemical is normally converted into another without any unneeded byproducts being formed. A new type of guiding protein was discovered during studies by Dr. Norman Lewis and associates at Washington State University on the biosynthesis of lignin, a major component of wood and other biomass resources. This guiding protein acts by specifically orienting the chemical substrate such that the enzyme can perform only one specific chemical reaction. This discovery is important to studies on lignin formation and may be relevant to numerous other biological processes. This biological strategy may also be applicable to the development of chemical catalysts leading to industrial processes that do not produce harmful byproducts.

Regulation of Photosynthesis in Bacteria. Three central metabolic functions in photosynthetic bacteria--photosynthesis, carbon fixation, and nitrogen fixation--are coordinately regulated. A signal/signal transduction pathway has been identified by Dr. Robert Tabita of Ohio State University that regulates the rate of the three metabolic functions. The identification of a single gene that can regulate three critical physiological processes is a major step in understanding the genetic regulatory machinery of bacteria.

BES FY 1997 Funding: $10.5 million
Number of BES Projects 81 (7 Laboratories, 68 Universities, 5 USDA, 1 Industry)

Program summary book index reference:
FY 1996 Energy Biosciences: Photosynthesis, Membranes or Ion Transport, Plant Metabolism and Biosynthesis, Carbohydrate Metabolism, Lipid Metabolism, Plant Cell Wall Development

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X			X	X	X								

RADIATION MATERIALS SCIENCE

The scope of The Office of Basic Energy Sciences (BES) research in radiation materials includes synergistic relationships between neutron, proton, and ion irradiation with defects, composition, and physical and mechanical behaviors in metals, ceramics, intermetallics, polymers, and semiconductors. Emphasis is on surface modification, modeling of radiation induced damage, cascade formation, property changes, design of radiation-resistant materials, irradiation induced stress-corrosion cracking, changes in grain boundary microchemistry, crack tip phenomena, and evaluation of spallation neutron and high energy proton damage.

There are 71 nuclear power reactors in the U. S. that are over 20 years old. The time-dependent radiation induced embrittlement of aging steel containment vessels and structural members defines a critical safety and environmental problem for these on-line facilities. Their continued safe operation requires a better predictive "early warning" or "retirement for cause" model for their behavior. There are three additional distinct motivations for BES activities in radiation materials sciences: (1) The many-generation safe containment of radioactive wastes requires valid predictive models for their time-dependent degradation under conditions including self-irradiation, heat, and the time-dependent production of radio-decay products; (2) The development of fusion reactors will require an understanding and a modeling of the radiation induced behavior of insulator and first wall component candidate materials such as silicon carbide, high-chromium ferritic-martensitic steels and vanadium; and (3) The energetic-ion-induced surface modification and implantation of metals, ceramics, polymers, and semiconductors is a continuously evolving science as well as an important technology that in turn underpins all energy conversion and conservation technologies.

Integration activities occur through the Energy Materials Coordination Committee and the annual Radiation Materials Sciences Contractor Meeting. Research at Oak Ridge National Laboratory (ORNL) is collocated with related work supported by the Office of Fusion Energy Sciences and the Nuclear Regulatory Commission (NRC). Research at Pacific Northwest National Laboratory (PNNL) is collocated with related work supported by the Electric Power Research Institute (EPRI).

SUCCESS STORIES

Correlating Radiation Damage in Fission Reactors with Predicted Behavior in Fusion Environments. The BES effort in fusion materials under the Mansur group at ORNL has developed an understanding of how transmutation generated helium affects swelling and phase stability and has successfully demonstrated swelling resistant alloy design for fusion applications. It has also developed, in partnership with the Fusion program, isotopically alloyed injector foils in order to obtain fusion-reactor-representative helium levels in materials irradiated in mixed spectrum fission reactors. Furthermore, a combination of theoretical modeling and strategically designed experiments has been used to develop the understanding required to use the extensive materials radiation effects database obtained from experiments in fission reactors to predict performance under fusion conditions. This understanding has also been employed in the design of radiation resistant alloys that offer improved performance relative to conventional materials.

Low Temperature Irradiation Embrittlement of Pressure Vessel Steels. Although it has been conventionally accepted that neutrons are the source of radiation damage in nuclear reactors, it was demonstrated under research supported by both BES and the NRC by the Mansur group at ORNL that pressure vessel steel embrittlement may be caused by gamma radiation induced atomic displacements. This matter is now being further pursued in a jointly supported effort by BES and the NRC. It has now been shown that embrittlement at temperatures of around 50^oC is relatively insensitive to damage rate over about five orders of magnitude in neutron flux. Embrittlement is also insensitive to the neutron spectrum in the sense that embrittlement is a response mainly to atomic displacements and not to the energy of the neutrons producing them.

Understanding Failure Modes of Radioactive Waste Storage Containers. The ability to predict the long term effects of radiation on the physical integrity of nuclear and radioactive waste containers requires a better fundamental understanding of the effects of irradiation on materials and more realistic predictive models. Recent work using simultaneous electron microscopy and ion irradiation experiments by the Rehn group at Argonne National Laboratory has shown that the impact of just a single high-energy ion on a surface surprisingly disrupts tens of thousands of near surface atoms and leads to the formation of surface craters and holes. It is important to understand this behavior for devising optimal hosts and storage containers.

Extended Creep Life for Fusion Applications. A low-swelling iron alloy known as AD9" was developed by the Mansur group at ORNL for cladding in liquid metal fast breeder reactor. Utilizing an understanding of the detailed relationship between irradiation effects in metals, metal microstructure, swelling, and creeps, the group developed an alloy toughened with many fine precipitates that would resist swelling pressures and creep. This alloy is now being applied to efforts to develop radiation-resistant materials for fusion reactors and for the lifetime extension of commercial power reactor structural components such as pressure vessels. It has lead Fusion Energy Sciences supported research to an extension of the creep life of type 316 stainless steel at 700^{o}C by over 1000 times by tailoring the microstructure to include several types of precipitates.

High Energy Ion Beam Processing of Polymers. High energy ion beam treatments have led to typical improvements in the hardness of soft plastic materials up to several times that of steels. The process developed by Lee at ORNL involves irradiation of polymer using energetic heavy ions, which leads to the transformation of the tangled polymer chains into a highly cross linked three-dimensional network structure. In contrast to earlier work on cross-linking with electron beams and gamma rays, which causes only relatively modest changes in hardness, this new approach produces large increases in hardness and a corresponding increase in wear resistance. Desired surface mechanical properties can be produced by tailoring the degree of cross-linking and depth of modified layer by appropriate choice of ion species, ion energy, dose, and fluence.

New Understanding of Irradiation Assisted Stress-Corrosion Cracking. Irradiation assisted stress corrosion cracking has been explained by Bruemmer at PNNL in terms of chromium depleted grain boundaries. Major solute diffusion parameters were measured and calculated in austenitic stainless steels at temperatures below 500^{o}C. Calculated diffusivity parameters were shown to be in accord with high-temperature, thermal-diffusion experiments. This BES work is now receiving further support from the EPRI.

BES FY 1997 Funding: $4.5 million
Number of BES Projects: 7 (4 Laboratories, 3 Universities)

Program summary book index reference:
FY 1996 Materials Sciences: Materials Sciences: Radiation effects, Point defects, Ion beam mixing, Stress-corrosion, Radiation: Electrons, Radiation: Gamma ray and Photons, Radiation: Ions, Radiation: Neutrons, Theory: Defects and Radiation Effects

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
				X				X		X	X	X	X

ROCK MECHANICS, FRACTURE, and FLOW

Rock mechanics, fracture, and fluid flow encompasses research on the response of rock to stress and the role of fluid flow as a cause and/or effect. Rocks are hosts to energy resources including coal, hydrocarbons, and geothermal energy, and they are the principal sites for energy storage as well as waste disposal in natural or engineered underground spaces. The prediction and interpretation of rock response offers unique challenges because the scales involved range from the microscopic to hundreds of kilometers and from seconds to geologic times. The properties of rock are dominated by extreme heterogeneity, pressure dependence, the presence of natural fracture systems, and the coupling between thermomechanical properties, fluid flow, and geochemical processes.

Integration between projects funded by the Office of Basic Energy Sciences (BES) and technology offices is achieved by interactions of investigators in shared laboratories, workshops and project reviews, exchanges between the Department of Energy (DOE) program managers, and joint facility/tools development. A recent facility advance includes the Office of Fossil Energy (FE)/BES development of novel rock mechanics/materials testing capabilities at Sandia National Laboratories. DOE national laboratory and university projects also address basic research elements of interest to technology programs that are supported by partnerships and consortia with industry. The integration of BES, technology offices, and industry is exemplified by a joint the Office of Energy Efficiency and Renewable Energy FE/BES development of core-based methods for in situ stress measurements and a joint EE/BES call for FY98 R&D proposals on rock drilling under the Small Business Innovation Research Program (SBIR).

SUCCESS STORIES

Prediction of Fracture Networks and Faults. Research at Stanford University, Northwestern University, and national laboratories is focused on the evolution of fracture networks and major fault systems. Fractures and faults are the most important conduits or seals for fluid and chemical transport in geologic systems. A combination of field observations and laboratory experiments at Stanford under Profs. Pollard and Aydin were used to develop quantitative mechanical models for the growth of discrete fractures and multiple fracture systems. Research by Prof. Rudnicki at Northwestern University and at national laboratories is focused on the hypothesis that some faults and the attendant shearing along narrow bands are the result of instabilities in constitutive behavior associated with micromechanical changes in rocks under stress. This basic research at Stanford University, Northwestern University, and DOE laboratories is the foundation of parallel applied research and reservoir interpretations between the same institutions and major oil producers including Chevron, Mobil, Amoco, and Conoco oil companies with funding from the FE National Petroleum Technology Office.

Imaging Porespaces in Sandstones. DOE-supported investigators at Brookhaven National Laboratory (BNL), Los Alamos National Laboratory (LANL), Sandia National Laboratories (SNL), State University of New York at Stony Brook (SUNY/SB), and the Mobil Exploration and Production Technology Center have been recognized in both the basic and applied research communities for their three-dimensional imaging of porespace in sandstones. The connectivity of porespace in rocks that form oil and gas reservoirs is central to understanding how formational fluids move through and interact with basin rocks. At SNL and SUNY/SB, a new technique adapted from biologic research, based on scanning confocal laser microscopy, has been developed to image connected porespace illuminated by fluorescent epoxy injected into reservoir sandstones. At BNL, a new technique suitable for intact reservoir drillcore, based on synchrotron x-ray microtomography, circumvents problems with averaging of image features in conventional methods. This technique is equally suitable for in-situ high-resolution imaging of pore structure and surface roughness. The porespace information is used in a joint program for improved oil recovery with LANL and Mobil, supported by FE and the Office Energy Research Office of Computation and Technology Research.

BES FY 1997 Funding:	$4.6 million	
Number of BES Projects:	37	(17 Laboratories; 20 Universities)

Program summary book index reference:
FY 1996 Geosciences Research: Geophysics and Earth Dynamics, Rock Mechanics, Fracture, and Fluid Flow

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
				X	X			X	X		X		

SOLAR PHOTOCHEMICAL ENERGY CONVERSION

Solar photochemistry research explores fundamental photochemical processes aimed at the capture and conversion of solar energy. This research program encompasses organic and inorganic photochemistry, electron and energy transfer in homogeneous and heterogeneous media, photocatalysis, and photoelectrochemistry. The photosynthetic reaction center is studied as a model for the design of efficient, photoinduced charge separation in biomimetic/photocatalytic assemblies. The research provides the foundations for future solar technologies in which light-induced, charge-separation processes will convert light energy to chemical energy in such applications as the production of alcohols from carbon dioxide, hydrogen from water, or ammonia from atmospheric nitrogen. Molecular-based photoconversion systems can also effect light to electrical energy conversion, although such systems face stiff competition in the near term from solid state, semiconductor photovoltaic solar cells. A strong interface with solar technology programs exists at the National Renewable Energy Laboratory (NREL) where investigators supported by the Office of Basic Energy Sciences (BES) and the Office of Energy Efficiency and Renewable Energy (EE) share laboratory space and equipment.

<u>SUCCESS STORIES</u>

<u>Artificial Photosynthesis</u>. Plants convert sunlight into chemical energy by the process of photosynthesis and this process has long tantalized researchers to find ways of mimicking plants to tap renewable solar energy. Under BES support, researchers Gust, Moore, and Moore, at the University of Arizona, have recently produced a model system that successfully mimics natural photosynthesis. The new model system converts the energy from light into a proton motive force which can be used in a number of energy utilization strategies. Light striking donor-acceptor molecules, imbedded in a balloon-like, liposomal membrane, induces charge separation in the molecules with the positive charge toward the outside of the membrane and the negative charge toward the inside. In response to this charge separation, protons are shuttled across the membrane by freely diffusing quinone molecules. In so doing, the separated charges in the donor-acceptor molecules are neutralized and the donor-acceptor molecules are free to repeat the process. The net result is energy storage in the form of an unequal number of protons on opposite sides of the membrane and is called the proton motive force. In ongoing work, the proton motive force stored in the liposome is being harnessed to provide a continuous source of chemical energy.

<u>Photoelectrochemistry at Interfaces</u>. Fundamental research at NREL, under the direction of Art Nozik and supported by BES, was focused on understanding electron injection into semiconductors from photoexcited dyes attached to their surface. The electron injection was found to generate a sufficient potential difference between the titania semiconductor and the counter electrode that lithium ion conduction could be facilitated. Furthermore, by coupling this knowledge with previous experience in electrochromic devices, investigators were able to take advantage of the lithium ion transport by coupling the titania to a transparent tungsten oxide. The lithium ions moved through the titania and into the tungsten oxide converting it into the colored lithium tungsten bronze. The extent to which the tungsten oxide is converted into the bronze is dependent on the intensity of the sunlight falling on to the dye sensitized titania. This research formed the basis of a jointly funded program to exploit these findings described in the following story. In addition, Monsanto is very interested in developing and marketing photochemical solar cells based on the dye substituted titania with NREL=s assistance.

<u>A New ASmart@ Window</u>. Smart windows conserve energy by changing their transmission properties in response to changes in the intensity of daylight. Existing smart windows require an external power source which is costly in retrofitting buildings. Recent research conducted at NREL by Brian Gregg's research team funded by BES, the Energy Research Office of Computational and Technology Research, and the EE Office of Building Technologies has resulted in the invention of a photoelectrochromic cell that combines two existing technologies: electrochromic windows and dye-sensitized solar cells. In the photoelectrochromic cell, a dye-sensitized, semiconductor film, converts daylight into electrical energy providing the voltage necessary to change the color of an electrochromic film. This eliminates the requirement of a separate power source. Envisioned applications for the new technology range from smart windows to light-addressable displays.

BES FY 1997 Funding:	$12.8	
Number of BES Projects:	65	(18 Laboratories; 47 Universities)

Program summary book index reference:
FY 1996 Chemical Sciences: Solar Photochemical Energy Conversion

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossill Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
			X	X		X							

SUPERCONDUCTIVITY

Basic research is performed on the theory, synthesis, processing, structure, and physical properties of high temperature superconducting materials including the discovery of new classes of superconducting materials. Research into the development of improved superconductors that can be used in the generation, transmission, utilization, and storage of electric power using high-T_c superconductors contributes to the efficient utilization of energy. The Office of Basic Energy Sciences (BES) research is coordinated with the Office of Energy Efficiency and Renewable Energy (EE) and the Office of Defense Programs (DP) through the Subcommittee on Superconductivity of EmaCC. The MatTech Communications Group on Superconductivity, which includes DOE, DOD, NSF, NASA, and NIH, is chaired by Dr. William Oosterhuis, BES. About 20 collaborations in this area exist between national laboratories and industrial concerns. The publication, *High-Tc Update*, is devoted to the rapid dissemination of information on superconductivity. This publication, supported by BES, has 2,500 direct subscribers and is visited 6,000 times per month on its web site. Both BES and EE superconductivity research is co-located at Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Los Alamos National Laboratory (LANL), and Oak Ridge National Laboratory (ORNL).

SUCCESS STORIES

Superconducting Quantum Interference Device (SQUID). BES supported scientist John Clarke and his colleagues at LBNL have developed the most sensitive magnetic flux detector of any kind available, constrained only by its inherent quantum limitations. This device measures magnetic fields on a minute scale. Although SQUIDs are based on physical principles known for many years, practical applications became feasible only with the advent of the high-T_c materials. Current applications include the detection of magnetic signals generated by various organs in the human body. Applications to non destructive testing of materials and geophysical exploration are presently being developed.

Rolling-Assisted Biaxial Textured Substrates (RABiTS). Under joint sponsorship by BES and EE, Drs. David Norton, David Christen, and John Budai at ORNL have developed a process for fabrication of a metallic tape that is superconducting at liquid nitrogen temperatures with a critical current density, at last report, of more than 1 megampere/cm^2. A current density of this magnitude is necessary for practical use of these new materials. To accomplish this, the RABiTS procedure was developed which enables the superconductor to posses a high degree of crystalline grain alignment in all directions, thus enabling larger superconducting currents.

Pairing Mechanisms in High Temperature Superconductors. The pairing of charge carriers in a superconductor is a necessary condition for the occurrence of superconductivity. The cause of this pairing in high temperature superconductors is not well understood. Recent experiments by Dr. Z.X. Shen at Stanford Synchrotron Radiation Laboratory (SSRL) have indicated that the pairing may be due to collective excitations of the electronic spin system. This new understanding, if confirmed, may lead to large scale applications of high temperature superconductivity, because the fundamental understanding might provide new ways to exploit the unusual properties of these materials.

Vortex Physics in High Temperature Superconductors. With the development of high temperature superconductors, a new field of investigation--that of magnetic vortices or ›vortex matter⁼--has emerged. Magnetic fields stronger than a lower critical field, penetrate superconducting films as an array of vortices, each consisting of exactly one quantum of magnetic flux surrounded in the plane perpendicular to the magnetic field by circulating supercurrents that extend radially for a few hundred nanometers. It is becoming clear that these vortices exhibit many interesting phenomena as they interact with each other and with externally applied fields. These phenomena include various ›frozen⁼ states in two-dimensional lattices, which melt or become ›glassy⁼, and are driven by the application of an electric field with the dissipation of energy, or are ›pinned⁼ by lattice defects which preserves the superconducting electric current. Much of the early work has been done at Argonne National Laboratory led by George Crabtree and V. Vinokur. An R&D 100 Award was recently given to Crabtree and Ulrich Welp for the development of a magnetic flux imaging system, which enables investigators to see clearly the structure and motion of these vortices.

BES FY 1997 Funding:	$18.6 million	
Number of BES Projects:	80	(52 Laboratories; 28 universities)

Program summary book index reference:
FY 1996 Materials Sciences: Superconductors: Ceramics; Metallic; Polymeric

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
				X	X			X				X	

WELDING and JOINING SCIENCE

Welding and joining are critical fabrication technologies that are used extensively in all energy, automotive, environmental, and electronic technologies. Weld failures are the most frequent reason for unscheduled and sometimes catastrophic outages in power plants with the cost of replacement power often exceeding $1 million dollars per day. Welding represents 10 percent of the cost of construction and 20 percent of the maintenance costs for a 500 megawatt fossil-fueled electric power plant. Welding and joining science is supported by both the Engineering Sciences and the Materials Sciences programs under the Office of Basic Energy Sciences (BES). The work scope includes understanding the microstructure and defects that develop as a consequence of temperature gradients; solid state phase transformations in weld heat affected zones; thermal processes as applied to gas metal arc welding; molten metal droplet formation; plasma and arc physics; laser welding of automotive aluminum alloys; time-resolved X-ray absorption spectroscopy to directly determine rate of transformation of one phase to another phase under the highly-nonisothermal conditions that prevail during welding; welding of Al, Ti and thin plates; coupling welding science and fracture mechanics modeling in response to the Northridge California earthquake experience; and critical issues in the non-welding joining of ceramics and dissimilar materials.

Integration activities occur through the Energy Materials Coordinating Committee, the Welding and Joining project under the distributed Center of Excellence for the Synthesis and Processing of Advanced Materials, and BES supported research in welding that is co-sited with Fossil Energy (FE) and Energy Efficiency and Renewable Energy (EE) supported work at Oak Ridge National Laboratory (ORNL). In addition, work on joining of silicon carbide is of special interest to the FE/Advanced Research and Technology Development Program, and investigations on joining of Continuous Fiber Ceramic Composites are of particular interest to the EE/Industrial Technologies Program.

<u>SUCCESS STORIES</u>:

<u>Development of Model for Inclusion Formation in Welds</u>. S. A. David and co-workers at ORNL and T. DebRoy and co-workers at Pennsylvania State University have developed a model for metal-oxide inclusion formation in steel welds that is based on the thermodynamics and kinetics of oxide growth in a steel melt. This is regarded as a major breakthrough in this area, which was once considered to be an intractable problem. These inclusions are very important because they radically change the properties of the weldment. This model enabled the design of improved consumable welding electrodes and the selection of welding process parameters that leads to improved weld quality.

<u>Weld Microstructure Model Developed</u>. T. Zacharia and co-workers at ORNL have developed the first model to predict directionally solidified grain structures in weld fusion zones in aluminum-silicon alloys. It correctly predicted which grain orientations would grow at the expense of other orientations. Since the grain structure of the weld fusion zone has a strong bearing on potential weld failure, predicting the grain structure is critical to the control of the welding process to achieve strong welds. This model has been applied in an Office of Naval Research Project and through recently completed Department of Energy (DOE)/Defense Program CRADAs.

<u>Three-Dimensional Weld Simulation Model Developed</u>. A three-dimensional model, WELDER, which takes into account both heat transfer and fluid flow in welding was developed by T. Zacharia, S. A. David, and co-workers at ORNL. The model is capable of predicting weld pool shape and temperature distribution in the heat affected zone. The model was applied to predicting the three-dimensional thermal history in single pass welds. This led to CRADAs with General Motors for welding advanced lightweight automotive materials and with Concurrent Technologies, a manufacturer of computer hardware and software located in Cincinnati, to develop WELDER further as an industrial tool for weld design and development.

<u>Demonstrated Feasibility of Electron Beam Welding Thick Steel Sections</u>. The feasibility of electron beam welding of thick section steel was demonstrated and, for the first time, a thorough analysis of the microstructure gradation within the heat-affected zone was carried out using weld parameter computer simulations. This research by S. A. David and co-workers at ORNL was applied, through a collaboration with the Chicago Bridge and Iron Company and the Office of Fossil Energy, to evaluate

high power electron beam welding of thick sections of 3% Cr -1.5% Mo -0.1 % V alloy steel, a composition previously developed for applications in fossil energy systems.

Model to Predict Microstructures in Single-Crystal Superalloy Welds Used in Advanced Turbines. The first mathematical model that describes and predicts the microstructural evolution in the fusion zone of welds in single crystals was developed by S. A. David and co-workers at ORNL. It successfully describes the experimentally observed microstructures in single-crystal nickel-base superalloys that are now used in advanced turbine systems for power generation and aircraft engines.

Established Mode of Solidification and Morphology of Ferrite Phase in Austenitic Stainless Steel Welds. A coupled thermodynamic and kinetic model by S. A. David and co-workers at ORNL was developed to describe the stabilities of the ferrite and austenite phases in stainless steel welds. This work included identification of the effects of controlled residual elements on improving the creep rupture properties, changes in weld composition, and mechanisms for both the high and low temperature embrittlement in stainless steels. Stainless steel welds are used extensively in power generation systems, petrochemical and chemical industries, and in the manufacturing of stainless steel hardware.

Gas Metal Arc Welding Research Used by Industry. The use of pulsed current gas metal arc welding (GMAW) has increased dramatically over the past five years due to the increased availability of better invertor power supplies. T. W. Eagar and co-workers at the Massachusetts Institute of Technology (MIT) have modelled the weld bead and examined ways to change the size and improve the efficiency and weld quality. John Deere and Company has used the MIT data to reduce weld fumes and increase weld quality without increasing cost. MIT will continue to work with John Deere to exchange research data for industrial issues. Idaho National Engineering and Environmental Laboratory (INEEL) has also been working to automate GMAW by better diagnostics and control circuits. This technology has been transferred to General Motors, Ford, and Chrysler.

BES FY 1997 Funding: $2.85 million
Number of BES Projects: 7 (5 Laboratories, 2 Universities*)

* includes two industrial collaborants under Partnered University-Industry Grant Program

Program summary book index references:
FY 1996 Engineering Sciences: 03-A and 03-B
FY 1996 Materials Sciences: Welding

Interactions (Xs) of BES research areas with DOE Energy Resources Programs and directly with U.S. Industry

Transportation Technologies		Seven Industries of the Future		Renewable & Utility Technologies		Building Technologies		Fossil Fuel Technologies		Fission Energy Technologies		Fusion Energy Technologies	
EE/OTT	Industry	EE/OIT	Industry	EE/OUT	Industry	EE/BTS	Industry	FE	Industry	NE	Industry	ER/FES	Industry
X	X	X	X		X			X	X				