FY 1987 ACCOMPLISHMENTS

OFFICE OF BASIC ENERGY SCIENCES

MARCH 16, 1988

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INTRODUCTION

Each year, the Office of Basic Energy Sciences (BES) compiles 30 to 40 "accomplishments" representative of the research being carried out under the program. For 1987, relevant accomplishments have been grouped to identify the rapid responsiveness of the program to the breakthrough in late 1986 in superconductivity and to illustrate the breadth of activity involving Basic Energy Sciences' Major User Facilities. Other accomplishments include I-R 100 awards, and sharing in a Nobel prize.

NOBEL PRIZE IN CHEMISTRY

Professor Donald J. Cram of the University of California, Los Angeles (UCLA), a long-time Basic Energy Sciences principal investigator, shared in the 1987 Nobel Prize in Chemistry this past year. The Prize was awarded to Professor Cram, Dr. Charles J. Pedersen of DuPont and Professor Jean Marie Lehn of the Louis Pasteur University for developing new chemical methods for recovering scarce metals and purifying common metals using much less energy than in the past.

Professor Cram's research is providing new insight into the chemistry of selectively combining molecules which can "tie up" a valuable metal in the presence of other common ones in solution and allow the new chemical combination to be removed. The novel substances prepared by Cram's research team can bind molecules as well as metals and can be designed to mimic the highly specific activity of enzymes, the remarkable catalysts that are essential to all forms of life. Thus, in addition to the applicability of Cram's work to recovery of scarce metals and purification of waste streams, the principles he has discovered also have widespread implications for the understanding of many processes that occur in nature. A Basic Energy Sciences investigator also shared in the 1986 Nobel Prize in Chemistry.

SUPERCONDUCTIVITY

Last year was important in the development of high-temperature superconductors. Although superconductivity was discovered in 1911, applications to date have depended on cooling with liquid helium. At the end of 1986, a breakthrough occurred in the temperature limit and newly developed "high-temperature" materials have been found which superconduct above the boiling point of liquid nitrogen. Liquid nitrogen is much cheaper and easier to use than liquid helium. To take advantage of the discovery of the new class of high-temperature superconductors, the Office of Basic Energy Sciences has supported research addressing scientific and technical obstacles to the use of the new materials in technologically important systems. The BES research program is addressing fundamental questions about the mechanism by which the new high-temperature materials become superconducting, the key to finding even better new materials. The program also is addressing the synthesis of new materials to expand their range. Following are five accomplishments in this area. BES Major User Facilities involved in these efforts are highlighted.

1. DOE LABORATORIES TAKE LEAD ROLE IN HIGH TEMPERATURE SUPERCONDUCTOR RESEARCH

Following the announcement by European workers late in 1986 of a superconductor with the transition temperature of 35° Kelvin, researchers at Argonne National Laboratory began an intensive study of the synthesis, characterization, and properties measurement of these new exciting materials. The 95° Kelvin superconductor of yttrium-barium-copper oxide material was made in February promptly after the discovery of this material by the superconductivity group at the University of Houston (not supported by DOE).

Neutron scattering studies with this material at the **Intense Pulsed Neutron Source (IPNS)** have provided the <u>definitive results on the structure of these "high temperature" superconducting ceramic materials</u>. Especially important was identifying the positions of oxygen atoms in the structure. The yttrium-barium-copper oxide material has "wrinkled" parallel planes of copper and oxygen atoms carrying the superconductivity. In collaboration with Brookhaven National Laboratory and Ames Laboratory of Iowa State University, these research results were being used in mid-1987 to develop current carrying "wire". Ames Laboratory has used expertise developed with earlier superconductors to understand the critical current behavior and Brookhaven Laboratory will use previously developed techniques to fabricate required forms of this brittle ceramic material. The wide variety of resources available within the DOE National Laboratories continue to play a vital role in understanding and developing these materials.

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2. PHOTOEMISSION STUDIES OF THE HIGH T_c SUPERCONDUCTOR YTTRIUM-BARIUM-COPPER OXIDE

Early 1987 saw an explosive growth of research activity into the properties of a class of materials which show superconductivity at high temperatures, as high as 95° Kelvin in the case of yttrium-barium-copper oxide.

The mechanism responsible for the superconductivity in these materials is still not understood and several different theories have appeared in the literature. Amongst these theories have been several calculations of the effects of different lattice atoms of the energies or velocities of electrons in these oxides. In low temperature superconductors the superconductivity is determined by the interaction of the electrons through the vibrations of the atoms in the lattice, a mechanism known as "electron-phonon coupling."

By illuminating the superconductors with light from the National Synchrotron Light Source (NSLS) it is possible to excite the electrons from the different atoms and determine their energies or velocities within the material. Studies of the superconductor yttrium-barium-copper oxide show that the electrons do not have energies as high as the calculations would suggest. The disagreement between experiment and the theoretical calculation suggests that either a very unusual version of the "electron-phonon coupling" mechanism or a new physical mechanism is responsible for the superconductivity in these materials. This work was done in collaboration with workers from AT&T Bell Laboratories and Temple University. It was one of the first reported photoemission studies of the high temperature superconductors and the unusual results have now been confirmed by other groups.

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3. IMPORTANCE OF RARE EARTH AND ISOTOPIC SUBSTITUTIONS IN SUPERCONDUCTORS

At Los Alamos National Laboratory, substitution of the rare earth, gadolinium, for yttrium in yttrium-barium-copper oxide barely affected its superconductivity. At Oak Ridge National Laboratory, the substitution of holmium, another of the rare earths, supported this observation. These results were consistent with the understanding that superconductivity is related to copper-oxygen planes and chains that do not include rare earth or barium ions.

Most of the rare earths have been substituted into the yttrium-barium-copper oxide material without destroying its superconductivity. Such substitutions are important to the development of a theory for these high temperature superconductors and, of course, there is the possibility that substitutions may raise the transition temperature even higher. There are indications of such increased transition temperatures from work at Lawrence Berkeley Laboratory (LBL) involving the successful substitution of praseodymium.

In other studies at LBL, substitution for the oxygen isotope O^{18} has confirmed the lack of an isotope effect in the yttrium-barium-copper oxide material, a result that strains the currently held theory of superconductivity; in the lanthanum-strontium-copper oxide material, however, an isotope effect was found.

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4. STRUCTURAL AND MAGNETIC EXCITATIONS IN HIGH TEMPERATURE SUPERCONDUCTORS

Progress in this field and the development of new materials call for a much better understanding of the microscopic physics underlying the superconductivity phenomenon. Specifically, one would like to know what is special about these materials which makes them different from other solids.

To probe the microscopic excitations within these materials, researchers at Brookhaven National Laboratory (BNL), in collaboration with groups from MIT and Tohoku University in Japan, have studied lanthanum-strontium-copper oxide using neutron scattering techniques at the **High Flux Beam Reactor (HFBR)**. In these experiments, neutrons penetrate the center of a single crystal and are scattered. By analyzing how they are scattered, it is possible to deduce the nature of the intrinsic atomic excitations in the material.

Experiments have revealed two distinct new phenomena. First, certain atomic vibrations involving the oxygen atoms are quite "soft". That is, oxygen atoms move with very little restoring force. This is true even at temperatures where superconductivity occurs. Currently, these "soft modes" are thought to be quite important to the high temperature superconductivity property.

Even more striking behavior is found in the magnetism. Specifically, the BNL-MIT-Tohoku University collaborators found that in the pure lanthanum-copper oxide material, the copper oxide sheets exhibit a novel type of magnetic order at quite high temperatures. The novelty resides in the fact that even though the material is ordered over long distances, the magnetism fluctuates rapidly in time. This behavior is unprecedented in these kinds of materials and leads to a number of questions to be explored: Is this behavior essential for superconductivity? Is the mechanism responsible for superconductivity magnetic in origin? What is the interplay between the soft vibrational modes and the magnetic excitations? Work in this exciting area continues.

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5. SOLUTIONS OF THE MAGNETIC ELIASHBERG EQUATIONS FOR HEAVY ELECTRON SUPERCONDUCTORS

Superconductivity has been attributed to a coupling of pairs of electrons called "Cooper pairs." The cause of this coupling in simple metallic superconductors is due to the vibrations of the atomic nuclei. The coupling mechanism responsible for superconductivity in another class of materials, known as "heavy electron" materials, has not yet been identified. Heavy electron materials are those where, to properly characterize their electronic properties, the electrons in them are assumed to be more massive than normal electrons. Calculations using DOE's large computers suggest that the superconductivity in heavy electron materials is due to a different phenomenon than atomic vibrations. However, using this new mechanism and equations [Berk-Schrieffer Eliashberg (BSE)] that should describe the phenomena produced inconsistent results, making clear that a more realistic description of the electronic structure and dynamics in the system was required. Although the electron energies can be calculated to very good precision, the required dynamics cannot.

It was realized, however,that a suitable result for the dynamics could be extracted from neutron scattering data. Even so, it has still been necessary to simplify the electron energy structure results to make the solution of the BSE equations tractible. The solutions of the BSE equations for a heavy electron superconductor like UBe_{13} required the full power of the CRAY II.

The results of the calculations by Argonne National Laboratory scientists were consistent with the new mechanism postulated. The superconducting transition temperatures obtained were in rough correspondence with the measured values. Thus it has been possible to describe semi-quantitatively the superconducting properties of the heavy electron materials.

There is evidence now that the mechanism active in the high temperature oxide superconductors may not be entirely due to the atomic vibrations mechanism; one might well inquire whether the new mechanism could be involved in these ceramic-like materials. With the appropriate neutron scattering data on the high temperatures materials, it will be possible to apply the approach used here to test the mechanism involved.

MAJOR USER FACILITIES

Basic Energy Sciences Major User Facilities provide a unique national resource for forefront research. Their availability to a wide range of researchers from academia, industry, and other government laboratories makes them especially valuable to the Nation. As illustrated by the accomplishments identified in the **SUPERCONDUCTIVITY** section above, the national laboratory structure and the availability of BES's Major User Facilities have been critically important to the ability of the BES program to quickly redirect research when the need arises. Accomplishments in other areas making use of these facilities also are presented here. The particular facilities involved in the accomplishments presented here are highlighted.

6. FIRST SUCCESSES IN HIGH RESOLUTION X-RAY HOLOGRAPHY OF BIOLOGICAL MATERIAL

A major step has been taken toward the goal of making three dimensional images of microscopic biological objects by x-ray holography. It was shown that x-ray holograms can be recorded at a high level of detail with reasonable exposure times using soft x-rays. This result allows successful numerical reconstruction of the image from the recorded data and makes it possible to make holographs using wet samples in an atmospheric environment.

A considerable number of x-ray holograms were recorded in late 1986 at the **National Synchrotron Light Source (NSLS)** x-ray ring. The best recordings are of granules about 1 micrometer in diameter from a rat's pancreas.

This research involved a collaborative effort among scientists from Lawrence Berkeley Laboratory, IBM, State University of New York's Stony Brook campus, and the University of California at San Francisco.

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7. NEW X-RAY MICROPROBE ACHIEVES 10 MICRON RESOLUTION AND WIDE APPLICATION

A resolution of better than 10 microns, with a high enough intensity to measure trace concentrations of atomic elements, has been obtained using a new x-ray microprobe designed by scientists at the Lawrence Berkeley Laboratory. In tests conducted at the Brookhaven National Laboratory, the new microprobe measured the concentration and spatial distribution of many elements quickly and simultaneously in a sample area of less than 100 square microns. When the x-rays struck a sample, elements in the sample fluoresced, yielding characteristic spectral lines which were then detected. Millionth-of-a-gram quantities of elements from potassium to zinc were easily measured within 300 seconds.

The ultra-high resolution that enabled the new microprobe to bring x-rays into such a crisp focus was made possible by the fabrication of unique mirrors. In experiments at the National Synchrotron Light Source, an intensity of 100 million photons per second has been achieved in a 10 micron diameter focal spot. Similar results have been achieved at the Stanford Synchrotron Radiation Laboratory.

Unlike electron microprobes, the new x-ray probe does not require that samples be placed in a vacuum. Consequently, it permits a wider variety of samples, including living biological specimens, to be studied.

Geologists, biologists and materials scientists have already made preliminary measurements with the instrument. Uses already made of the microprobe have included a medical study to reveal the distribution of toxic concentrations of trace elements in biological tissue, and a study of ceramics to locate internal cracks and flaws. A wide variety of samples, including ceramic zinc oxide, single red blood cells, and melanoma cancer sections are being scanned to study the application of this new x-ray microprobe to other scientific fields.

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8. CRYSTALLIZATION STUDIES OF CATALYST MATERIALS USING NEUTRON DIFFRACTION

Zeolites are porous crystalline materials which are extremely important as catalysts in many chemical processes, most notably in the petroleum industry. The geometries of the pores in zeolites restrict the sizes and shapes of molecules which can be accommodated during a chemical reaction. Varying the nature of the zeolite and its geometry makes possible extraordinary control of the type of reaction product that a catalytic process will yield. Understanding the principles and mechanisms involved in crystallizing zeolites is the key to making systematic advances in the discovery of new zeolite materials. The process of crystallization of a zeolite used in converting natural gas to methanol and coal into gasoline in the presence of "template" molecules is being investigated at Argonne's **Intense Pulsed Neutron Source (IPNS)** using small angle neutron diffraction. "Template" molecules are molecules of predetermined size and shape that, if incorporated into a crystallizing zeolite, will control its pore size.

Neutrons offer a unique advantage in the study of crystallite nucleation and growth since they can distinguish between hydrogen and deuterium atoms; this permits isotopic labeling of the organic template to establish how it gets incorporated.

The **IPNS** results have effectively elucidated the mechanism involved. A gel is formed from a silicate solution. The template molecules are incorporated directly into the amorphous particles upon gel formation, setting up an embryonic structure for the zeolite being studied. The zeolite develops by direct crystallization of the solid gel particles. These experiments constitute a joint research project involving scientists from the Australian National University and Argonne National Laboratory.

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9. IMAGING TECHNIQUE PROVIDES SPATIAL DISTRIBUTION OF MOLECULAR DISSOCIATION PRODUCTS

A new technique has been developed at the **Combustion Research Facility (CRF)** in conjunction with a visitor from Cornell University that makes it possible, with a single laser pulse, to determine the three-dimensional spatial distribution of the dissociation products when a molecule is fragmented. The technique yields direct information on angular and speed distributions and hence details on the dynamics and time scale of the dissociation event itself.

The new imaging method is applicable to a host of chemical problems including those in combustion. It may be most useful in the detection of products of molecular beam experiments, a research area for which the 1987 Nobel Prize in Chemistry was awarded.

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10. TRANSURANIUM ELEMENTS USED FOR CANCER THERAPY RESEARCH

The **High Flux Isotope Reactor (HFIR)** and **Transuranium Processing Plant (TPP)** at Oak Ridge National Laboratory have been used to produce two isotopes used by the Oak Ridge Associated Universities in National Cancer Institute-supported cancer therapy research. Einsteinium-253 and fermium-255, two alpha emitters of 20.5 day and 20.1 hour half-lives respectively, are bound to monoclonal antibodies which have the ability to specifically direct these radionuclides to malignant sites. Alpha emitters are ideal for cancer therapy because their entire radiation energy is confined within a very small volume. Therefore, the number of alpha "strikes" required to kill a cancer cell is much lower than for other types of radiation. It is also important that alpha emitters to be used in cancer therapy have a reasonably short half-life so that the radiation dose to the patient can be better controlled.

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11. SYNCHROTRON RADIATION USED TO IDENTIFY SEMICONDUCTOR FILM DEFECTS

Scientists from the Lawrence Berkeley Laboratory (LBL) and Hewlett-Packard Laboratories have collaborated in applying synchrotron x-ray scattering techniques to study structural defects in thin gallium-arsenide (GaAs) films grown on silicon (Si) by various techniques. This semiconductor system is of both basic scientific interest and intense technological interest as a means of monolithically integrating GaAs and Si devices and as a means of obtaining GaAs substrates with large areas.

Application of this new technique revealed several important features in the GaAs system which had not been seen before using traditional in-lab characterizations. These features result from specific and identifiable structural defects. GaAs films grown by different techniques under varying conditions are being studied to correlate these structural defects with growth conditions. Such work is critical for improving the production of these important semiconductor materials for better electronic and optoelectronic devices. X-ray scattering experiments were performed at the Stanford Synchrotron Radiation Laboratory (SSRL) on a beamline owned jointly by LBL, EXXON and SSRL.

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OTHER BASIC ENERGY SCIENCES ACCOMPLISHMENTS

The first eleven accomplishments presented reflect the current importance of research in the superconductivity area and the broad usefulness of BES' unique Major User Facilities. Additional accomplishments representative of the balance of the program are presented below.

12. LIQUID METAL THERMOACOUSTIC ENGINE

A sound wave is usually thought of as consisting of pressure and velocity oscillations; always present with the pressure oscillations are small temperature oscillations. The interaction of all these oscillations produces a rich variety of "thermoacoustic" effects which are so small they are never noticed. Under the right circumstances, however, they can be harnessed to produce powerful heat engines, heat pumps, and refrigerators. A project at Los Alamos National Laboratory combining theoretical and experimental studies of thermoacoustic effects in liquid sodium has produced a novel heat-driven electrical generator having no moving mechanical parts.

Although the liquid-metal acoustic engine is less efficient than some other engines, such as steam-turbine driven generators, it has the advantages of simplicity and no moving mechanical parts, an advantage in systems requiring high reliability. It has a higher efficiency than thermoelectric generators, and hence may eventually replace them in satellites and other applications where reliable generation of electrical power is extremely important.

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13. X-RAY LASER AND ITS APPLICATION

In 1984, Princeton University scientists conducted the first demonstration of a laboratory-size x-ray laser. In 1986 the laser delivered enough energy per pulse to produce photographic images, and in 1987 the first microscopic images produced by any x-ray laser were actually obtained using the Princeton University laser. For their work on x-ray laser development, Princeton University and Princeton X-Ray Laser, Inc. were awarded one of the 1987 I-R 100 awards which are presented annually by Research & Development Magazine to the 100 most significant new technical products in the world.

Laser-based x-ray microscopy offers the prospect of observing, for the first time, the insides of living cells, including the distribution of chemical elements within a cell. Imaging live cells is likely to produce important discoveries in cell biology which, in turn, could have impact on medicine. While the wavelength of the Princeton laser is still too long to image cells, work towards developing a shorter wavelength x-ray laser is in full progress.

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14. MATHEMATICAL DESIGN METHODS IMPROVED FOR SYSTEMS WITH MEMORY

Many systems, as they operate, retain a "memory" of their recent past. In particular, they may "remember" how their properties changed with time to reach their current state. For instance, a system's "state" may depend on its previous history, for example, whether its current temperature was reached by cooling or by heating. The mechanical lag in steering wheels is another familiar example. The "state" of the front wheels of a car, i.e., where they are pointing, depends not only on how far the steering wheel has been turned, but also on the "history," i.e., the direction in which it was last turned.

Thus a system with "memory" might be changed from its existing state to either of two resultant states for the same value of an external control setting. This phenomenon is called hysteresis. Hysteresis may be used to advantage as a memory element or, on the other hand, hysteresis may play havoc with attempts to calculate and predict the future behavior of a system.

Important systems exhibiting hysteresis include magnets, used in electric motors and generators; chemical reactors; viscoelastic materials, such as automobile tires; mechanical systems with backlash, such as robot arms; and computer memories. Until now, the design and numerical simulation of these systems either simply ignored hysteresis, incurring a penalty in the integrity and economics of the design, or involved very costly and imperfect computations based on inadequate approximations to this phenomenon.

Recent research at the University of Maryland on engineering systems with hysteresis has resulted in the formulation of a new mathematical description of hysteresis, which, in turn, has led directly to new powerful calculational methods for incorporation in routine design and simulation algorithms. Of particular significance are the simplicity of the new methods and their applicability to systems and materials with a wide range of characteristics.

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15. VIDEO SYSTEM ALLOWS OBSERVATION UNDER BLINDING CONDITIONS

In many industrial and experimental processes high quality video images are prevented by a bright glow emitted by those processes. Examples are the electric welding arc, plasma processing of materials, and combustion flames. In particular, welders would like to have a precise view of the welding pool, the electrode and the solid-liquid interface: the information gained from such a view is important to the welder in assuring the quality of the weld seam. Of equal importance is a high quality image of the weld arc and its environment for automated welding systems; on-line processing of the image and the use of the extracted information for automated control of the welding process can assure a high quality, reliable weld.

At the Idaho National Engineering Laboratory, a system producing such high quality video images in the presence of extremely bright backgrounds has been developed. It uses the latest advances in optoelectronics and signal (image) processing. The importance of this achievement has been duly recognized by the engineering community. Recently the I-R 100 Award winners included the inventors of this imaging system. Research & Development Magazine, an International Journal of Research, Development and Quality Assurance, holds an annual international competition for this award. The one hundred award winners are selected on the basis of their technical significance, uniqueness, and usefulness. In the last round, the winners were chosen from among more than 10,000 world-wide candidates.

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16. TECHNIQUES DEVISED TO ENHANCE DISTILLATIONS FROM MANY MIXTURES

Combinations of two liquids which show a minimum or maximum boiling point at some fixed composition intermediate between those of the pure components are called azeotropes. Distillation is a process that separates two liquids by heating them to the boiling point of the more volatile component which then boils off leaving the other component behind. Distillation of azeotropes is a more complex matter; the azeotropic composition will be the one that either boils off or remains behind, depending on the composition of the initial solution.

The usual procedure for azeotropic distillation is to introduce a third component which will affect the relationships between the solution composition and boiling points in a helpful way. This added component, referred to as the "entrainer", will thus allow separation of the two original liquids to a greater extent than the azeotropic limit. A research effort at the University of Massachusetts has yielded a simple, rigorous method for determining feasible entrainers and has developed and published a technique for establishing the operating conditions in complex columns involving azeotropic distillations. The resulting savings in energy and capital investment are expected to continue for many years as the new method is incorporated into introductory textbooks and handbooks in chemical engineering.

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17. ROCK SALT RESEARCH GUIDES DESIGNS FOR OIL AND NUCLEAR WASTE STORAGE

Rock salt is an impure form of the substance most familiar as table salt or sodium chloride. It occurs sometimes in large deposits which in recent years have been shown to be very valuable for a variety of applications. Two uses important to the Department of Energy are for the storage of crude oil and possibly for the storage of nuclear waste.

One of the long-term Basic Energy Sciences projects has been concerned with the mechanical behavior of rock salt. The project was completed last year. It showed how the walls of mines and caverns formed in rock salt slowly move over periods of years. The mechanisms of this slow creeping of the salt were identified and certain impurities were shown to have large effects. The results have proven critically important for two disparate applications. First, they made possible a reliable model for projecting the long-term stability of structures being used for the strategic petroleum reserve. Second, they have proved essential in interpreting tests at the Waste Isolation Pilot Project in New Mexico which is being used to explore methods for the storage of defense wastes.

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18. GRAIN BOUNDARY STRUCTURAL CHANGES

Advanced transmission electron microscopy has revealed that in iron-gold alloys, gold migrating to grain boundaries causes the boundaries' structure to change from that of pure iron. Similar research is in progress on grain boundaries in ceramics where a structural transformation is observed, although it is of a different kind than in iron. This finding of a change in the <u>structure</u> of boundaries is important.

Many materials of technological importance consist of a collection of small, individual crystallites called grains. The boundaries between these grains are known to be important in determining the properties of the materials as a whole. In addition, it is known that impurity atoms, called solutes, can find their way to the grain boundaries and cause changes in the boundaries' properties. These changes can have a significant effect on, for example, the mechanical properties of materials and render them brittle and susceptible to fracture at low stresses. However, until now it has not been known why the properties of the boundaries are so dramatically affected. This study at Cornell University has shown, for the first time, that solute segregation actually causes a change in the <u>structure</u> of grain boundaries in both metals and ceramics.

If grain boundary structural changes can be linked to changes in properties in a quantitative way, it will become feasible to design materials with specified boundary structures which give rise to desirable bulk properties for both mechanical and electronic applications.

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19. ADVANCED TECHNIQUES FOR ATOMIC MODELING

Predictions of the behavior of materials based on mathematical models of atomic interactions can be very valuable in supporting experimental results and, especially, in uncovering new phenomena. The "Embedded Atom Method" (EAM) is a significant advance in atomic modeling; it allows treatment of more complex and interesting problems than currently used methods. Furthermore, this new method involves no increase in computational complexity over existing methods of calculation.

Evaluating the EAM led to good correlation with experimental data; further, the potential to treat situations too complicated for previous methods became clearly evident. Recent applications of the EAM have been directed toward the understanding of dislocation dynamics, including the effects of association of hydrogen atoms with dislocations, the calculation of stresses necessary to initiate brittle crack propagation, and the calculation of the segregation of alloying elements to free surfaces, among others. For ranges of variables where experimental data were available or where other more common methods of calculations were valid, agreement was observed. The EAM, however, provided additional, critical insight to these topics as well. These topics are of current interest in many BES programs; the EAM thus has great potential for contributing to a wide variety of ongoing research activities.

It is clear from results to date that the EAM represents a major advance over existing methods for atomic modeling. Already, investigators from more than one-half dozen universities and national laboratories are applying the EAM to additional scientific problems.

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20. REACTION DYNAMICS EXAMINED BY THEORY AND EXPERIMENT

The positive interplay between theory and experiment was illustrated recently by a theoretical re-interpretation of data obtained from an experimental measurement of the chemical reaction dynamics of an important combustion reaction. In the reaction that takes place between excited oxygen atoms (O) and hydrogen molecules (H_2), the final products are OH radicals and hydrogen atoms (H). If D, deuterium, a heavier isotope of hydrogen, is substituted for one of the H atoms in the hydrogen molecule, the final products can be either OH + D or OD + H. Based upon theoretical models of chemical dynamics, the ratio of hydrogen to deuterium (H/D) can be predicted. The ratio observed can be used to deduce whether the mechanism of the reaction involves insertion of the O atom into the bond between the hydrogen and deuterium atoms or abstraction of either the hydrogen or deuterium atom.

A recent experimental study by Professor Bersohn at Columbia University has shown that the OD/OH ratio, which should be identical to the H/D ratio, predicted by J. Muckerman of Brookhaven National Laboratory, is qualitatively correct but has a severe quantitative discrepancy. Muckerman repeated the calculation and found that the lifetime of a reaction intermediate, on a femtosecond (10^{-15} seconds) timescale, is critical to the correct interpretation of the mechanism of the overall process. Bersohn's experimental results, and Muckerman's theoretical calculations both clearly support an insertion mechanism.

Theoretical understanding of combustion reaction chemistry is an important component in combustion systems design and control technology. This accomplishment resulted directly from interactions brought about through Basic Energy Sciences' combustion research program.

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21. ION SCATTERING BY SINGLE ATOMS IN CRYSTALS DEMONSTRATED

It was shown at Oak Ridge National Laboratory, for the first time, that ion scattering by single atoms can be studied in the solid state. In the experiment performed, a very high quality thin crystal of silicon, 14 millionths of a centimeter thick, was aligned precisely to allow passage of a proton beam without striking the silicon atoms. The network of highly symmetric silicon atoms, with proper orientation, presented a channel to the incoming proton beam through which it could travel without striking the silicon atoms. It was possible to measure the number of protons in the incoming beam that were deflected at particular distances from the central axis of the channel. The new results can be used to determine interatomic energy relationships in crystals and to ascertain energy transfer mechanisms of atoms or ions passing through crystals.

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22. RATES AND MECHANISMS OF RADICAL-RADICAL REACTIONS

Free radicals are highly reactive species with one or more unpaired electrons. In flames their concentrations can become large enough for reactions between two radicals to be important. At present, theoretical studies provide the <u>only</u> means of determining the rates and mechanisms of these kinds of reactions at combustion temperatures.

Recently at Argonne National Laboratory, two reactions between atomic hydrogen with both formyl (HCO) and peroxyl (HO_2) radicals, have been studied theoretically. In both cases the calculated room temperature rate constants are in good agreement with experiment and, in addition, predict the temperature dependence of both the rate and product ratio of the processes. The calculations show that certain processes that are relatively unimportant at room temperature become significant at flame temperatures.

It is becoming increasingly clear that modern theory combined with advanced computers can provide new insights into chemical kinetics. In particular, calculations provide a predictive capability in important areas where experiments are not presently feasible.

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23. LASER CONTROLLED ENERGY TRANSFER OBSERVED

In a study designed to understand and increase the efficiency of rare gas excimer lasers, scientists have, for the first time, actually controlled the amount of energy transferred from one atom to another during the "collision" process. The transfer begins with the formation of a two-atom collision complex. The complex exists only for an immeasurably short time while the two atoms are undergoing "collision".

Professor Keto at the University of Texas found that the incident laser wavelength used to add energy to an atom corresponds to the interatomic distance during collision. He used this knowledge to effect excitation of the colliding atom at any particular distance by simply tuning the excitation wavelength. With such selectivity, a substantial increase in our understanding of, and ability to control, reaction transition complexes whose formation is a prelude to ensuing chemical reactions is likely.

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24. TUNNELING CONTRIBUTION TO CHEMICAL REACTION RATES MEASURED EXPERIMENTALLY

The first unambiguous demonstration of the effects of "tunneling" on the rate of a chemical reaction was presented this past year. Tunneling is a purely quantum mechanical phenomenon that has been observed in a number of experiments but which has never been demonstrated unambiguously to influence the rate of a chemical reaction. By carefully measuring the influence of temperature and isotopic mass on the rate of reaction of hydrogen molecules with oxygen atoms, Professor Robert J. Gordon and his students at the University of Illinois at Chicago have shown that quantum mechanical tunneling can indeed influence dramatically the rate of a chemical reaction. In the future, the effects of tunneling will have to be considered in accurate models of combustion processes. The demonstration of tunneling required a comparison of the experimental data with accurate quantum mechanical calculations. These calculations had already been performed by scientists at Emory University, the University of Minnesota, and Argonne National Laboratory.

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25. NEW MEMBRANES REMOVE NITROGEN FROM NATURAL GAS

A new series of membranes has been discovered which are more permeable to nitrogen than to methane. The new membranes were prepared at the University of Texas at Austin in an effort aimed at improving the heating value of natural gas supplies contaminated with nitrogen.

The new membranes are the first to prefer nitrogen over methane with a permeation rate large enough to be of practical value. They remove the undesired nitrogen without a reduction in the pressure of the natural gas. Existing membranes suitable for processing large quantities of gas unfortunately are permeable to methane and reject nitrogen and the resulting product stream would have to be recompressed before it could be used.

The preference for nitrogen by these membranes is sufficient to permit upgrading of lower quality natural gas supplies having 10% nitrogen to a usable gas with under 5% nitrogen.

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26. ACCELERATOR RESEARCH FOR INERTIAL FUSION APPLICATIONS

Heavy Ion Fusion Accelerator Research (HIFAR) is carried out using a special kind of accelerator, the induction linac, to assess its suitability as a "driver" for generating electricity based on the concept of inertial confinement fusion. In this approach to fusion, an induction linac would be used to deliver intense beams of charged atoms, called ions, in a few billionths of a second to a small fuel capsule. The capsule needs to be compressed to fusion conditions, releasing substantially more energy than that contained in the beams from the linac. For efficient electrical power generation, this process must occur several times each second.

The major feasibility problems facing this application of induction linacs are being addressed through a sequence of experiments of increasing scale and sophistication. At Lawrence Berkeley Laboratory, fabrication was completed early in 1987 on the second element in this sequence. Called the Multiple Beam Experiment (MBE-4), this accelerator apparatus addresses some of the physics issues associated with the low energy, electrostatic portion -- the first section -- of the induction linear accelerator. An initial series of tests demonstrated, for the first time, that simultaneous acceleration and current amplification of the ion beams can be carried out with adequate beam control and no perceptible degradation of beam quality. Comprehensive testing of MBE-4 is under way to optimize its performance and to ascertain the range of beam parameters available for stable operation.

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27. NEW COMPUTER MODEL TO PREDICT COMPONENT LIFE UNDER COMPLEX CYCLIC LOADINGS

A new unified model describing elevated-temperature fatigue has been developed at Stanford University. The processes represented in the computer code correspond closely to the physical mechanisms elucidated recently in the basic research of many investigators. A key feature is that failure is fundamentally incremental, and is predicted in terms of the initiation and growth of cracks occurring by a succession of local fracture events. This model successfully predicts a variety of materials behavior and failure phenomena.

The methodologies which stem from this model can be used to increase the reliability of structural components, permit more optimal design and materials selection, determine rational inspection intervals, eliminate premature retirement of components, minimize the need for extensive material testing programs, and facilitate the introduction of new alloys. The model represents a new level of integrated, scientific understanding of the very complex process of fatigue in metals and alloys.

Components of the model can be used for predicting fracture of structural ceramics, including the effect of flaws (especially small flaws) on their strength, thereby providing a basis for design and material selection for new, complex, toughened ceramics. Since industry does not have a sufficient experience base with these materials, a capability for credibly predicting their structural reliability will be important for their commercial utilization.

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28. HIGH SENSITIVITY DETECTION AND CHARACTERIZATION OF AMERICIUM IN AQUEOUS SOLUTION

Chemists at Argonne National Laboratory (ANL) have observed fluorescence from americium (III) in aqueous solution and have developed a thousand-fold improvement in detection sensitivity for this element in comparison with standard optical methods. Detection of as little as one-hundred-millionth-molar solution concentrations (in the parts per billion range) is possible using "Time-Resolved Laser-Induced Fluorescence" (TRLIF) which may also provide the means to identify the chemical nature of the aqueous species. Information on the amounts and chemical forms of americium in ground water is essential for the licensing of certain nuclear waste repository sites because americium is expected to become the dominant source of radioactivity in such a site after 1,000 years. The anticipated solubility limits of americium in ground water are expected to be in the detection range of this method. This research result is being explored in collaboration with another ANL group under the auspices of the DOE Basalt Waste Isolation Program.

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29. DRILLING SHEDS UNIQUE LIGHT ON NEAR-SURFACE MAGMATIC PROCESSES

One of the most fundamental steps in understanding the nature of structures and processes in the earth's crust is examination of how magma (molten rock) has behaved as it approached the surface. The igneous rocks formed this way cover the great majority of the earth's surface. The best places for study of magma processes are often the sites of volcanoes which are recent from a geological perspective.

As one of the first activities under the national Continental Scientific Drilling Program, a research drilling project was completed in 1987 which took an approach new in the field of magmatic process studies. The approach was to sample subsurface portions of a very young igneous system before chemical and physical degradation has occurred. Four holes ranging in depth from 150 to 970 meters were drilled into the Inyo Domes chain, a 600 year old, 10 km long line of volcanoes that is the product of the most recent eruption of Long Valley Caldera, California.

Results of the study of the materials taken from these holes include: 1) a new model for subsurface porous flow degassing of magma to explain nonexplosive eruptions; 2) evidence that degassing controls crystallization; and 3) better understanding of the chemical zonation and mixing in silicic magna. Approximately 20 investigators at four DOE laboratories, several universities, and the U.S. and Canadian Geological Surveys have contributed or are contributing papers to the refereed literature reporting these results. Potential applications of results include improved understanding of thermal budgets of volcanic areas, volcanogenic ore deposits, and eruption hazards.

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30. NEW PHENOMENON OBSERVED IN PITTING CORROSION

It has recently been shown that light inhibits the nucleation of corrosion pits on nickel in brine solutions. The extent to which inhibition occurs depends upon light intensity. Increasing the power density of white light from a tungsten lamp by a factor of 5 reduced the number of pits that nucleate by more than 90%. This phenomenon has not previously been reported, but it is expected to have a major impact on how we describe the nucleation of pits on industrially important metals and alloys.

Corrosion costs the United States about $150 billion annually, and some of this loss is due to localized corrosion such as pitting attack. To avoid this form of corrosion damage, it is frequently necessary to use specially alloyed and expensive steels. Accordingly, considerable economic incentive exists to understand the cause of pitting corrosion and to develop lower cost, pitting resistant materials for use in ships, aircraft, and industrial systems. Pits nucleate at structural defects in the protective oxide film, whereas absorption of light involves the electronic structure; thus, this new observation provides direct evidence for coupling between structural and electronic defects on the surface. This observation has led to a new way of describing the nucleation of pits that is now being used to design new, pitting resistant alloys.

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31. CLIMATE MODELLING WITH SUPERCOMPUTERS

The availability of Energy Research supercomputer time has been directly responsible for improving the ocean models used in part to estimate possible CO_2-induced climate change. The first ocean models used were called "swamp oceans" and were simply two dimensional wet surfaces with no heat content that were a source of water vapor. The current ocean models are called slab or mixed layer oceans. The oceans are assumed to be a 50-70 meter deep slab or a layer of water with heat content but no ocean currents. The supercomputers have been used to develop the so-called real (or full) ocean models. Although these are still rudimentary, the models attempt to include bottom topography, wind driven and density driven currents, and other physical attributes responsible for the global ocean circulation and the interaction of the ocean and the atmosphere as they relate to possible global climate. The ocean models are still insufficient for quantitative forecasting.

What has been accomplished is the reduction in the error for calculating the January "Sea Surface Temperature" (SST) between two versions of the model. The SST error has been significantly reduced over most of the North Pacific and North Atlantic Oceans, especially in the central equatorial Pacific. This reduction in error in the tropical Pacific is extremely important for subsequent enhanced CO_2 experiments and will increase the significance of the results. The remaining SST errors in other regions are the targets of current testing.

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32. HYDROGEN METABOLISM IN ANAEROBIC BACTERIA

A project on anaerobic bacteria (bacteria that can only grow without oxygen) at the University of Georgia has recently provided insight into the biochemistry of these widely distributed organisms. Anaerobic microorganisms are pivotal in the energy and gas cycling in many environments lacking oxygen including swamps, mines, deep oceans, and digestive tracts of animals. Hydrogen is believed to play an important role in transfer of energy during the growth and life cycle of these organisms, and a detailed study of the enzymes known as hydrogenases that are responsible for the production and consumption of hydrogen in these critically important bacteria was undertaken.

Three forms of hydrogenase may be distinguished based upon the metal components present in the enzyme. These forms are the iron-containing (Fe form), the nickel-iron-containing (NiFe form), and the selenium-nickel-iron-containing (SeNiFe form). The genes for the structure of the NiFe form and SeNiFe form have been isolated. Analysis shows that while there are similarities in a few small parts of the hydrogenase molecule, the two forms are very dissimilar. Comparison of the NiFe and SeNiFe hydrogenase genes with a Fe hydrogenase gene shows that there is little if any similarity. As these differences in structure are likely related to differences in function, the biophysical and catalytic properties of the various hydrogenases are presently being studied to determine the precise role of each form in the metabolism of anaerobic bacteria. These results are important in the context of understanding energy cycling in the broad sense as well as in conceiving of any biotechnological developments of processes for producing hydrogen as an alternative fuel or industrial chemical.

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33. MODEL PLANT FOUND TO BE POWERFUL EXPERIMENTAL SYSTEM FOR PLANT RESEARCH

The small plant, Arabidopsis thaliana, of the mustard family has been given special attention recently at the Michigan State University/DOE Plant Research Laboratory. An international symposium was convened in 1987 at Michigan State University to discuss extensively the opportunities, advantages and techniques for utilizing this as a model system in higher plant research. Among the benefits offered by Arabidopsis are the small size of both the plants and the seeds (no need for large greenhouse or field space), the short life cycle of the plant, its simple chromosome structure and the small amount of DNA in each cell.

Arabidopsis has proven to be an excellent organism in which to find mutations, a fact that is being extensively exploited at the Plant Research Laboratory to investigate such phenomena as the response of plants to light, fat and oil metabolism, herbicide resistance and others. In the longer term, Arabidopsis may prove to be more important than being simply a useful laboratory organism. It has already been demonstrated that certain genes that have interest in an agronomic context can be isolated from Arabidopsis and subsequently transferred to crop plants where they are expressed. Hence Arabidopsis may be the vehicle by which useful genes are generated by mutation for later transfer and exploitation in crop species.

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34. ANALYTICAL SOLUTION OF LASER PROPAGATION MODEL HELPS IN BEAM FOCUSING

An analytical solution to a mathematical model of laser propagation through the atmosphere is providing new insights into the beam focusing problem. When a high powered laser propagates through the atmosphere, the air is heated and the diameter of the beam increases, causing loss of power density. This is the so-called "thermal blooming" problem. It may be possible to overcome this problem by focusing the beam so that it remains collimated as it propagates through the atmosphere. A mathematical model that governs the propagation of the laser beam has been solved numerically by researchers in the free electron laser optical science and technology program at Lawrence Livermore National Laboratory (LLNL). Though valuable, it is difficult to judge from this solution how changes in the physical parameters of the system affect the beam. Work at the Ames Laboratory, jointly undertaken with LLNL researchers, began to answer this question. An analytical solution to the LLNL mathematical model was developed at Ames. This solution agrees with numerical results in some trial cases. Obtaining the numerical results is quite time consuming, even on a supercomputer; thus a range of results obtained analytically is providing physical insight into the problem that otherwise would have required very large amounts of supercomputer time.

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35. CHARACTERIZATION OF POROUS CERAMIC MATERIALS

A new and powerful method (magnetic resonance relaxation analysis, MRRA) has been developed and applied at Northwestern University to characterize the pore size distribution in technologically relevant ceramic materials. In this approach, measurements are performed on a volatile liquid infused into the pores.

MRRA clearly indicates the presence of both small and large pores and that these are separated from one another by a distance greater than one micron. Non-uniformity on a micron scale is seen for the first time with this method, indicating processing flaws.

Every ceramic body is formed in a processing sequence which begins with a highly porous compaction of ultrafine ceramic powder. The manufacturer of higher strength ceramic materials requires the identification of non-uniform pore distributions that develop during the sinter-processing sequence. Some of the unique features of MRRA are that it is non-destructive, it can be used on almost any shape, it is sensitive to pore sizes in the range 30 to 10,000 angstroms, and it has spatial image resolution similar to that used in magnetic resonance imaging. This method can be directed to a particularly sensitive location in the ceramic body to determine otherwise hidden defects. The method can be applied quickly without the need of remote facilities such as for neutron scattering.

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36. NEW COMPOSITE MATERIAL USED IN RECORD SETTING MAGNET

Copper niobium (CuNb) composite materials were tested at the National Magnet Laboratory for high strength, high conductivity applications. The CuNb alloy, with a strength twice that of stainless steel and conductivity 70% that of pure copper had been prepared, cast, and rolled at Ames Laboratory at Iowa State University and extruded at Supercon, Inc. A major achievement with the composite material was the production of a high field pulse magnet which set a world record for the highest field ever generated, 68.4 Tesla, by a wire wound solenoid. A Tesla is a unit of magnetic field strength. The field attained was limited by the available energy: had the energy been available, the magnet would most probably have generated at least 75 Tesla.

Electrodes fabricated from CuNb material possess the best erosion resistance of all materials currently used in high current, high energy spark gaps. Consequently, possible applications include such areas as high current opening switches, solid armatures, current carrying rails of electromagnetic railguns, brushes and slip rings of compact homopolar generators, and electrodes for MHD power generators.

This is an example of an effective and on-going technology transfer from a National Laboratory, which designed and produced the alloy for high strength, high conductivity applications, to a small business which used alloy wires to produce the solenoid for magnetic applications.

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37. NEW MATHEMATICAL INSIGHT FOR SOLVING WAVE FRONT PROPAGATION PROBLEMS

A class of algorithms has been created and tested for following wave fronts whose speed depends on the curvature. This is the first accurate and reliable method for following this type of front motion, and is of great importance in a variety of physical phenomena, such as flame motion, crystal growth, and secondary oil recovery. In these problems, the front separating the two media (reactants and products, water and ice, oil and water) can become extremely complicated. Previous algorithms for solving these problems suffer from numerous drawbacks: 1) poor accuracy, 2) instabilities near sharp corners, 3) inability to follow complex topological changes, and 4) difficulty in going to higher dimensions. The success of these new algorithms, developed at the University of California, Berkeley, and the Lawrence Berkeley Laboratory, results from the realization that the problem is actually easier to solve in one higher dimension than the physical setting. Using the advanced technology for the numerical solutions of gas dynamics, it was possible to produce schemes of high accuracy. The simplest version of the scheme, which works in any number of dimensions, requires approximately 100 lines of computer code.

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38. SUPERCOMPUTER ANALYSIS OF SUPERNOVA 1987a DATA

Supernova 1987a was the first supernova explosion close to the earth in modern times. It was close enough to present a unique experimental test of our understanding of cosmology and astrophysics, and, serendipitiously, particle physics. Because it was unexpected, there was no preparation to observe this event; in fact some existing detectors which could have provided insight into the emissions from the explosion were not operating at the time.

The IMB high energy physics group operates a large volume neutrino detector in a salt mine under Lake Erie. The IMB experiment is a determination of the lifetime of the proton, and the detector's photomultipliers were tuned to discriminate against interference from solar neutrinos. Nevertheless, eight "astrophysical" neutrinos from the supernova were detected. Because of the Energy Research supercomputer time available to the IMB group, an effort to analyze the limited data collected was made and the results were very rewarding. Collaborating with the IMB group were the Universities of California and Minnesota. A new lower bound on the neutrino lifetime was established, 100,000 years; a new limit on the neutrino mass was set, 11 eV; and the number of neutrino species was found to be six or less.

The considerable significance of these fortuitous data and the analysis is the establishment of several new limits on important parameters of the Grand Unification Theory and the arrival times of the astrophysical neutrino emissions will help establish the sequence of events associated with supernova 1987a. The latter are not consistent with existing perceptions of supernova processes and require further theoretical development. The analysis would not have been attempted without access to a supercomputer.

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39. DEEP WELL SAMPLES SHOW WHEN NATURAL GAS IS AND IS NOT STABLE

At the temperatures and pressures characteristic of sediments several miles in depth, petroleum is unstable, that is, it undergoes chemical reactions and is converted to other products such as natural gas. Gas formed and trapped in very deep sediments is thought to constitute an enormous energy resource within the U.S. Some concern has developed, however, over whether there is a limit to the depths at which natural gas itself is stable. The deepest hole in sediments is currently 31,441 feet but the deepest gas production is from only 26,536 feet. The depth gap between deepest hole and deepest producer is the largest in the history of the oil and gas industry.

A research project funded by Basic Energy Sciences since 1979 has made three major contributions to predicting the stability of natural gas under the conditions encountered in deep sedimentary basins. First, a new technique was developed for determining the extent of the chemical reactions which could destroy natural gas at great depth. The tiny individual inclusions of gas were analyzed from a large number of samples of rocks from deep wells. The new technique is already being widely used in the oil and gas industry. Second, a sizable body of fundamental data was obtained which allows precise calculation of the extent of the chemical reactions undergone by natural gas over large ranges of temperature and pressure. Third, a convenient computer program was recently developed by researchers at the University of Tulsa; it allows industry scientists to use their own measurements from particular areas and wells to forecast the regions of stability for natural gas.

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40. EXTRACTION OF INDUSTRIALLY IMPORTANT METALS ADVANCED BY NEW CHEMISTRY

Scientists at Oak Ridge National Laboratory have discovered two novel combinations of reagents which permit highly selective extraction of metals from complex mixtures. In the first, cesium can be extracted from mixtures with metals such as sodium using a "crown" ether containing a bulky hydrophobic group. A "crown" ether has a molecular shape that visually resembles a crown, hence the name. The researchers had predicted from molecular structure theories that the particular system chosen would show high selectivity toward cesium. The crown ether was then synthesized for the first time at Texas Tech University. The extraction system may be valuable as a means of segregating cesium from nuclear wastes. Current techniques for recovering radioisotopes of cesium are cumbersome.

The second new system permits removal of copper and silver from mixtures with common metals such as iron. It involves a crown ether containing sulfur atoms in place of the customary oxygen atoms of the "crown". The reagent shows a thousand-fold preference for copper and silver over iron, maganese, cobalt, nickel, and zinc. The chemicals are reusable, and show potential for recovery of copper and silver from ores and mining waste streams. The significance of this work is that solvent extraction is used to obtain about one-third of all copper produced from ores in the U.S. and systems in current commercial use have great difficulty in isolating copper from iron.