

**FY 1989
ACCOMPLISHMENTS**

OFFICE OF BASIC ENERGY SCIENCES

MARCH 1, 1990

SOME EXAMPLES OF ACCOMPLISHMENTS
UNDER THE BASIC ENERGY SCIENCES PROGRAM
DURING 1989
MARCH 1, 1990

THE BASIC ENERGY SCIENCES (BES) PROGRAM SUPPORTS ABOUT 1,400 RESEARCH PROJECTS. THE FOLLOWING SELECTION OF ACCOMPLISHMENTS DOES NOT REFLECT THE FULL RANGE OF ACTIVITIES UNDER THE PROGRAM. IT DOES, HOWEVER, PROVIDE EXAMPLES OF HOW BASIC RESEARCH CAN CONTRIBUTE TO SOLVING A WIDE VARIETY OF ENERGY PROBLEMS. THE ACCOMPLISHMENTS IDENTIFIED ARE PRESENTED IN THREE SECTIONS:

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2. TECHNOLOGY TRANSFER, 1989 R&D 100 AWARDS, AND SMALL
BUSINESS INNOVATION RESEARCH ACCOMPLISHMENTS DURING
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THE FOLLOWING SUBPROGRAMS WERE MANAGED AND/OR FUNDED UNDER BASIC ENERGY SCIENCES DURING FISCAL YEAR 1989.

MATERIALS SCIENCES (MS)
CHEMICAL SCIENCES (CS)
ENGINEERING AND GEOSCIENCES (EG)
APPLIED MATHEMATICAL SCIENCES (AMS)*
ENERGY BIOSCIENCES (EB)
ADVANCED ENERGY PROJECTS (AEP)
SMALL BUSINESS INNOVATION RESEARCH (SBIR)**

* MANAGED BY THE SCIENTIFIC COMPUTING STAFF OF THE OFFICE OF ENERGY RESEARCH

** MANAGED UNDER ADVANCED ENERGY PROJECTS

FY 1989 BASIC ENERGY SCIENCES ACCOMPLISHMENTS

Section 1

Major Facilities Related Accomplishments During FY 1989

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8. **Depth Profiling of Interfaces Using X-Ray Reflectivity**
National Synchrotron Light Source (NSLS), Brookhaven National Laboratory: S. M. Heald and H. Chen (MS)

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FY 1989 BASIC ENERGY SCIENCES ACCOMPLISHMENTS

Section 1

Major Facilities Related Accomplishments During FY 1989

1. **Synchrotron X-ray Studies of Growth of Semiconductor Surfaces**
Stanford Synchrotron Radiation Laboratory (SSRL), S. Brennan; AT&T Bell Laboratories: P. H. Fuoss, D. W. Kisker, G. Renaud, and K. L. Tokuda; and Stanford University: J. L. Kahn (MS)

The first in-situ X-ray study of the growth of a semiconductor surface by organometallic chemical vapor deposition was carried out at the Stanford Synchrotron Radiation Laboratory (SSRL). The study was made of the growth of zinc selenide on a gallium arsenide surface. The experimental technique used low angle grazing incidence scattering of extremely bright X-rays.

Despite the technological importance of these types of semiconductor surfaces, little is known about the detailed mechanisms of the commonly used processes for preparing them. To obtain such information, it is necessary to actually observe the growth processes at the atomic level. Recently improved magnet technology provided a "bright" enough beam of X-rays to carry out the desired experiments. These initial experiments, involving the operation of a chemical vapor deposition apparatus in the X-ray beamline, have demonstrated the feasibility of using proven X-ray based analytical techniques to "see" structural details while the films are growing. These key experiments involved a collaboration among AT&T Bell Laboratories, SSRL, and Stanford University scientists.

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2. **Two-Dimensional Compressibility of a Metal Measured for the First Time**
Stanford Synchrotron Radiation Laboratory (SSRL); Lawrence Berkeley Laboratory: P. N. Ross and J. B. Kortright; IBM-Almaden Laboratory: O. Melroy, M. Toney, G. Borges, M. Samant; and University of Puerto Rico: L. Blum (MS)

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

The data obtained were used to calculate the two-dimensional compressibility of the monolayer (one-atom thick) lead film in contact with the silver surface. The lead film deposited on the silver surface is initially compressed about 1.4% relative to bulk lead; this compression increases to approximately 2.8% relative to the bulk when the applied voltage is high enough for the onset of multilayer deposition. The compression of the monolayer film produces stress between the lead and silver at the interface which, in turn, influences the structure and properties of the bulk lead deposit.

This research result and the technique used to obtain it are important for understanding thin film deposition processes and their control; such processes are widely used in fields such as electronics and corrosion resistant coatings.

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3. **Polarization and Resonance Properties of Magnetic X-ray Scattering**
National Synchrotron Light Source (NSLS), Brookhaven National Laboratory: L. Doon Gibbs and M. Blume; AT&T Bell Laboratories: D. R. Harshman, E.D. Isaacs and D. B. McWhan; Cornell University: D. Mills; Rice University: J. P. Hannon and G. T. Trammell; and the Institut Laue-Langevin, France: C. Vettier (MS)

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

To understand how polarization analysis opens the door for magnetic studies, consider a beam of linearly polarized X-rays incident on an array of magnetic atoms whose magnetic moments are arranged in a simple spiral. If the X-ray energy is far from an absorption edge of the target, then scattering theory predicts that the magnetically scattered component with linear polarization perpendicular to the scattering plane will come from that part of the magnetic moment produced by the spin angular momentum of the atomic electrons. The parallel-polarized component, however, will contain as well, a contribution due to the circulation of the atomic electrons in their orbits (orbital angular momentum). Thus, polarization analysis provides a way to identify and characterize the spin and orbital contributions to the magnetic moment—something which has not been possible before. Measurements have been made of both linear components of the magnetic scattering from holmium atoms by this technique, allowing for the first time a direct comparison of experiment with theory.

In other experiments, large resonant X-ray scattering has been discovered in holmium and in other materials. This unexpected increase in the intensity of the magnetic scattering has been explained as arising from electric multiple transitions from non-conduction to conduction band states. Thus, X-ray magnetic scattering is found to be sensitive to the detailed properties of the magnetic states of the material. Resonant magnetic X-ray scattering provides a valuable new spectroscopy of magnetic materials and because of the large enhancements, many new kinds of experiments are now possible with today's synchrotron sources.

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4. **Magnetic Excitations in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$** *
High Flux Beam Reactor (HFBR), Brookhaven National Laboratory: G. Shirane, H. Chou, T. Freltoft, T. Thurston, J. M. Tranquada, Y. J. Uemura, and K. Yamada; Massachusetts Institute of Technology: R. J. Birgeneau (MS)

It is now clear that magnetism and superconductivity are closely associated in the layered copper oxide compounds. In these compounds, an antiferromagnetic insulator is transformed into a superconducting metal by doping with electron holes. Considerable evidence has accumulated that the copper atoms retain their magnetic moments in the metallic phase. Thus, at a minimum, magnetism is an important indicator of strong electronic correlations in these materials, and it may yet prove to be crucial for electron-pairing in the superconductors.

Pioneering neutron scattering investigations of magnetism in the high T_c systems have been performed at Brookhaven National Laboratory beginning with La_2CuO_4 , the first compound for which large single crystals became available, and continuing on strontium-doped crystals. In the past year, these studies have been extended to the $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ systems, for which the maximum superconducting transition temperature is 90K at $x = 1$. Large single crystals with various oxygen contents have been grown by a group at the Institute for Molecular Science in Japan. Extensive neutron scattering measurements of magnetic excitations in these crystals have been performed in collaboration with researchers at the Massachusetts Institute of Technology. Samples with a low oxygen content exhibit three-dimensional magnetic ordering. Evidence of a very strong magnetic coupling between copper atoms within the CuO_2 layers, the common structural element of these compounds, is present. In contrast to the lanthanum compound, however, the interaction between nearest-neighbor pairs of CuO_2 planes turns out to be surprisingly strong, and the magnetic moments within a bilayer remain correlated well above the maximum temperature for three-dimensional order. Measurements on superconducting crystals reveal a dramatic change in the low energy magnetic excitation spectrum compared to that in the insulating samples. In fact, no magnetic scattering features in the superconductors, have yet been identified even though magnetic susceptibility studies indicate the correlated moments should be present. Work is continuing to better characterize the magnetic cross section in the superconductors.

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* Superconductor ceramic materials often are identified by their chemical compositions. Item 4, for example, is about $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, its molecular composition is 1 atom of yttrium, 2 atoms of barium, 3 of copper and $6+x$ atoms of oxygen. The expression "x" is a deviation from stoichiometry (a perfect molecule with no "vacancies"). Another term that arises is "1-2-3 compound" which refers to the ratio of the principal metal atoms in the system, e.g., 1 yttrium, 2 barium and 3 copper atoms in the example above.

5. **Intercalation Compounds: Implications for Advanced Battery Materials**
High Flux Beam Reactor (HFBR), Brookhaven National Laboratory;
University of Pennsylvania: J. E. Fischer (MS)

High capacity rechargeable batteries are likely to be important in future energy strategies and this research provides new insights into the selection of materials for batteries based on "intercalation" compounds. Ions intercalated (inserted) between layered structures at high temperatures create local distortions to the structure that stabilize the distorted structure when the temperature is lowered. Neutron diffraction at the HFBR was used to determine the local distortions for lithium inserted between layers of graphite and titanium disulfide. Graphite monolayers, which are essentially 2-dimensional, are quite deformable in their plane, resulting in short relaxation distances of the layers around the intercalated lithium and large strain energies. Conversely, the internal bonding of the sulfur-titanium-sulfur layers in titanium disulfide produces a much stiffer structure, longer relaxation distances for the layers and more diffuse strain fields. Estimates of the in-plane attractive interaction explain why the lithium carbide family of intercalation compounds goes through a sequence of undesirable staging transitions as lithium concentration changes, whereas lithium-doped titanium disulfide shows no phase transitions during electrochemical intercalation and deintercalation at 300K.

Many new battery technologies rely on intercalation (insertion or doping) of a mobile charge carrier (ion) into an inorganic lamellar or organic polymer electrode. Exciting new results demonstrate that phase transitions, which are detrimental to electrode life due to dimensional changes, can be controlled by proper selection of dopant and host material. This breakthrough provides a rational basis for selecting host materials for intercalation batteries. Furthermore, more recent data suggest that the same concepts may be applied to polymer electrodes.

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6. **Study of Reactions of OH Radicals Results in Improved Understanding of Alcohol Combustion**
Combustion Research Facility (CRF), Sandia National
Laboratory/Livermore: F. Tully (CS)

Alcohol fuels, both methanol and ethanol, are attractive alternative fuels to gasoline because they are less polluting and can be produced from domestic coal or biomass rather than from imported oil or gas. Their effectiveness in existing and new internal combustion engines is of critical concern and has prompted research on their combustion chemistry. The hydroxyl radical, OH, is a reactive molecular fragment always present in alcohol and other hydrocarbon combustion systems which contain both oxygen and hydrogen atoms. Studies of the reaction mechanisms of the hydroxyl radical with various alcohols have provided new, unanticipated information to help understand and control the combustion of alcohol fuels. The hydroxyl radical is a dominant, and perhaps the most dominant, reactive species in both alcohol and hydrocarbon combustion reactions although the reaction mechanisms are

different. Design of highly efficient combustion devices depends strongly on how well the different participating reaction mechanisms can be characterized and their relative rates specified. Thus experimental information on hydroxyl radical-alcohol reactions is critical to accurately model the processes involved.

Studies at the CRF, employing its unique capabilities to follow extremely rapid reactions under a wide range of experimental conditions, have now shown that the hydroxyl radical-alcohol reaction mechanism actually changes significantly with temperature. The change with temperature of the reaction rate is not "smooth". Instead, when the hydroxyl radical-alcohol reaction rate was measured over a temperature range from 300K to 800K, it underwent a dramatic shift around 600K. These studies at the CRF were characterized by an unusually high degree of accuracy for chemical reaction rate measurements and by an exceptional amount of ingenuity in the use of isotopic enrichment to sort out competing reaction mechanisms. The major surprise was the discovery that at high temperatures the hydroxyl radical-alcohol reaction constitutes a catalytic, chain mechanism for the conversion of alcohols to a particular class of hydrocarbons called alkenes. Thus in modeling a practical combustion system involving alcohol fuel, the subsequent combustion chemistry of the product alkene also must be included.

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7. Nature of the Charge Carriers in Electron-Doped Copper Oxide Superconductors

National Synchrotron Light Source (NSLS), Brookhaven National Laboratory: J. M. Tranquada, S. M. Heald, A. R. Moodenbaugh; Rutgers University: G. Liang and M. Croft (MS)

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

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

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* See footnote on page 4.

8. Depth Profiling of Interfaces Using X-Ray Reflectivity
National Synchrotron Light Source (NSLS), Brookhaven National
Laboratory: S. M. Heald and H. Chen (MS)

X-ray reflectivity measurements have been used to determine the depth dependent concentration profile of copper across a copper-aluminum interface with a sensitivity to copper concentrations of less than 1 percent and to a depth resolution of about 4 atomic diameters. Measurements made as a function of heat treatment of the interface revealed significant differences in the reactivity of copper/aluminum interfaces depending on the amount of oxygen present. These were made possible by the high resolution of the technique; previously when the reacted layer was thick enough to be observed by Rutherford Backscattering (RBS) or X-ray diffraction measurements, the differences disappear. Transmission Electron Microscopy (TEM) measurements also were hindered by the tendency of this system to react during sample preparation.

Interface interactions are important in a number of applications including advanced electronic and optical components. Using synchrotron radiation the X-ray reflectivity method can be applied to a wide variety of interface systems. It offers improved depth resolution over standard techniques such as RBS, and does not require the extensive and difficult sample preparation needed for TEM measurements. The penetrating nature of X-rays also allows the technique to be applied in situ to monitor the response of an interface to outside factors. Thus, the depth profiling information obtained from the reflectivity should provide an improved understanding of many technologically important interface systems.

FY 1989 BASIC ENERGY SCIENCES ACCOMPLISHMENTS

Section 2.

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FY 1989 BASIC ENERGY SCIENCES ACCOMPLISHMENTS

Section 2.

Technology Transfer, 1989 R&D 100 Awards, and Small Business Innovation Research Accomplishments During FY 1989

Technology Transfer

1. High- T_c Superconductor Technology Transfer Argonne National Laboratory: B. N. Dunlap (MS)

Argonne National Laboratory (ANL) has developed a technology for coating metal wires with malleable precursor elements of the high T_c superconductors that contain the rare-earth metal yttrium. When these wires are heated, the elements form the less malleable high T_c superconducting ceramic around the wires. These composites thus provide the mechanism for the fabrication of wires sufficiently long and strong for high T_c superconductor applications.

American Superconductor Corp., Cambridge, Mass., a company formed last year to commercialize new superconductors, has agreed to license this technology from Argonne. American Superconductor also has agreed to provide \$100,000 to ANL for research on other superconductor technologies. Argonne has one of the nation's largest superconductor research groups.

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2. Chemistry of Electrons in Organic Liquids Important for Superconducting Super Collider Electronic Detector Development Brookhaven National Laboratory: R. Holroyd (CS)

Hydrocarbon liquids are finding use in high energy physics experimental detectors. Ionizing particles passing through the detectors leave tracks of electrons and ions characteristic of the particle, its weight, energy, charge, etc. The properties of electrons generated by ionizing radiation in non-conducting organic liquids, e.g., benzene or hexane, have attracted the attention of high energy physicists designing new room-temperature liquid-phase electronic detectors. Information is needed on the properties of "free" electrons in hydrocarbons, particularly their motion in electronic fields and reactions with impurities, as well as radiation-induced decomposition of the hydrocarbon. For use in high energy physics detectors, the hydrocarbons need to be extremely pure: impurities such as oxygen and carbon dioxide must be reduced to the part-per-billion level to assure that electrons released in the tracks of ionizing particles survive long enough to be collected in the detectors.

Holroyd has recently been invited to speak at a number of workshops devoted to detector development, both here, for the Superconducting Super Collider (SSC), and abroad. He was visited recently by Carlo Rubbia, who is leading the development of a giant new dosimeter (referred to by physicists as a

calorimeter) at CERN. It will utilize 10,000 liters of a hydrocarbon (2,2,4,4-tetramethylpentane) supplied by Wiley Organics, Inc., of Ohio. As Wiley refines its purification procedures, Dr. Holroyd determines electron "lifetimes" in samples sent to him employing the Van de Graaff accelerator at Brookhaven National Laboratory. For the proposed SSC, radiation effects on hydrocarbons are of concern due to high radiation levels (up to 10^7 rads/year) in the detector areas. Hydrocarbons are decomposed by radiation into products including hydrogen and methane gases. The Brookhaven group has estimated that gas pressure buildup upon irradiation of hydrocarbons could amount to 5-6 atmospheres if no provision is made for venting. Another problem is that the electron's survival time is reduced by the decomposition products. These effects will be considered in design of detectors for the SSC.

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3. Ion Source Finds Application in Trace Explosive Detection Devices
Oak Ridge National Laboratory: G. L. Glish and S. A. McLuckey (CS)

A practical device for explosives detection is under development at the Oak Ridge National Laboratory. Based on research under the BES program, other DOE offices, other Federal agencies and private companies have undertaken development of a device able to detect trace gaseous components characteristic of explosive materials as well as trace gaseous pollutants in the environment.

This new device is based on an atmospheric sampling glow discharge ionization (ASGDI) source that ionizes trace polyatomic compounds in air for subsequent mass spectrometric analysis. A voltage difference of 400 volts between two electrodes creates ions from ambient air at low pressure which then react with the trace gaseous molecules to generate the ions of interest. These are analyzed by mass spectrometry.

The DOE Office of Safeguards and Security has funded the effort toward developing a device for explosives detection and the FBI and Food and Drug Administration have expressed interest in devices suited for their purposes. An exclusive license has been granted to the Finnigan Corporation in San Jose for the development of a commercial device for the detection of pollutants in the environment.

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4. Innocuous Metal Scavenger Molecules Designed, Synthesized, and Demonstrated
Argonne National Laboratory: E. P. Horwitz (CS)

Chemical compounds able to strip metal ions from acid streams have been developed which can subsequently be degraded using mild thermal or chemical treatment into innocuous substances: water, carbon dioxide, and phosphoric acid. These newly designed compounds are highly efficient stripping agents and will have broad application in the processing of highly acidic nuclear wastes and in decontamination of ground water. After serving their useful

purpose the molecules can be easily destroyed, thereby avoiding subsequent problems in recycling, storage, or disposal. The compounds have been dubbed TUCS, for Thermally Unstable Complexants. A patent application is in process, and several firms have expressed an interest in obtaining a license to produce these compounds on a commercial scale.

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5. **MAGIC Liquid Chromatography/Mass Spectrometry Interface Commercialized**
Georgia Institute of Technology: R. F. Browner (CS)

A new liquid chromatography/mass spectrometry (LC/MS) interface, dubbed MAGIC, for Monodisperse Aerosol Generation Interface for liquid Chromatography, has been developed. Importantly, the interface is compatible with traditional electron bombardment ionization so that mass spectra produced can be directly compared to extensive libraries of fragmentation patterns for unambiguous molecular identification. The eluent from the chromatograph is subjected to a rapid expansion which serves to both generate an aerosol of uniformly sized particles and reduce the pressure to that required for introduction into the mass spectrometer. This system has been commercialized by Hewlett-Packard Corporation as the "Particle Beam Interface" under an exclusive license. It made an immediate and major impact on the LC/MS market upon its introduction in late 1988 and is expected to achieve a sales volume of \$40,000,000 in 1990.

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6. **Nobel Prize Work Leads To Commercial Products For Serum Analysis**
University of California at Los Angeles: D. J. Cram (CS)

In 1987, Professor Donald J. Cram shared in the Nobel Prize in Chemistry for

"developing new chemical methods for recovering scarce metals and purifying common metals using much less energy than in the past".

Professor Cram's research provided new insight into the chemistry of selectively combining molecules which can "tie up" a valuable metal in the presence of other metals in solution and allow the new chemical combination to be removed. The novel complexing agents developed can bind molecules as well as metals and can be designed to mimic the highly specific activity of enzymes. The principles discovered by Prof. Cram have widespread implications for the understanding of many processes that occur in nature.

These complexing agents have been adapted by Technicon Instruments Corporation of Tarrytown, NY, for quantitative analysis of sodium and potassium in serum, an important measurement for proper electrolyte balance. Such analyses are conducted routinely in the clinical laboratory.

Routine analysis for sodium and potassium ions in serum has been conducted by either flame photometry or the use of ion specific electrodes (ISE). Both of these techniques are labor intensive and require special equipment. ISE requires high-cost maintenance. Technicon Instruments Corporation has recently announced commercial availability of their ChromoLyte reagent for colorimetric analysis for K^+ in serum samples, and a similar reagent for Na^+

colorimetric analysis for K^+ in serum samples, and a similar reagent for Na^+ is expected to be available soon. With these new reagents, quantitative analysis for alkali ion content of serum can be conducted by conventional colorimetric methods commonly used for most other clinical analyses. Ease of use and cost effectiveness are major advantages of these new reagents for clinical analyses.

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7. Innovative Approach to Hazardous Waste Treatment

Illinois Institute of Technology Research Institute (IITRI): J. Bridges (AEP)

In the early '80s, the Office of Basic Energy Sciences sponsored exploratory research on a process using electromagnetic radiation to heat in situ large volumes of shale and tar sands deposits. The process was based on an ingeniously designed system of antennas so configured that the "microwave oven" type heat would evolve only in the designated volume. While the falling world prices of crude oil made the method unattractive for the extraction of oil from shale and tar sands, an application for hazardous waste treatment was recently developed by the engineers at IITRI who originally invented the system. This patented process, called "In Situ Radio Frequency Decontamination" treats the waste in place, without excavation, at a low cost estimated at between \$50 and \$90 per ton of soil treated. . Weston, a major company active in hazardous waste removal, concluded an exclusive licensing agreement with IITRI. In a press release the company has characterized the process as "a significant breakthrough in reducing the cost of treating many of the nation's hazardous waste sites."

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8. Welding Vision

Idaho National Engineering Laboratory: H. Smart; and Massachusetts Institute of Technology: D. Hardt (EG/E)

A recently developed welding vision system has attracted the interest of the US Army. The system developed at INEL about three years ago lets the welder see clearly the weldpool through the glare of the welding arc. The direct view of the pool helps the welder maintain the needed high quality of the weld itself. As reported previously, this instrument received the prestigious R&D 100 award. Now the US Army is supporting at INEL the development of software which will permit the welding vision system to be incorporated in a robotic welding cell at the Army's Rock Island Arsenal.

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9. Heat and Mass Input Controller

Idaho National Engineering Laboratory: H. Smart; and Massachusetts Institute of Technology: D. Hardt (EG/E)

A heat and mass input controller for gas-metal arc welding developed as a result of the collaboration between INEL and MIT is being installed on a robotic welding system at the US Navy's David Taylor Research Center (DTRC).

The controller embodies the basic knowledge of some of the relationships between the flow of the metal into the weld and the flow of heat away from the weldment on the one hand and the quality of the weld on the other hand. The ongoing recently established cooperation between INEL and DTRC aims at reducing defects in welding processes used in ship building.

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10. Data Network Congestion Avoidance
Lawrence Berkeley Laboratory: Van Jacobson (AMS)

The work of Dr. Van Jacobson on computer networking and its rapid exploitation was recognized in 1989 through an award from his Laboratory for excellence in technology transfer. Dr. Jacobson has developed a set of algorithms to control and avoid congestion on heavily loaded data transmission networks of computers. These procedures are already being utilized in the protocols in use on many of the important networks in the world. Before the implementation and deployment of the seven algorithms involved, these networks were observed to undergo catastrophic drops, as much as a thousand to one reduction, in data transmission rates when the data load passed a critical value. With the new procedures in place, the data rates maintain a smooth increase with load until the load nearly reaches the theoretical limit for the network.

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1989 R&D 100 Awards

11. INEL Simulation Software Finds Wide Acceptance in Mass Spectrometry Community
Idaho National Engineering Laboratory: D. A. Dahl, J. E. Delmore,
A. J. Applehans (CS)

An ion optics computer program which has found wide acceptance by both users and manufacturers in the mass spectrometry community has been developed at the Idaho National Engineering Laboratory. The ion optics program SIMION, for ion simulation, originally developed to support research in gas phase analytical chemistry at INEL, has become a standard tool used by scientists interested in understanding and using charged particle beams. The program enables the user to understand ion trajectories through complex potential fields with user defined boundary conditions. The program is easy to use in an interactive mode and provides extensive computer graphics to help build intuition and understanding in ion optical systems.

Over 200 organizations and individuals have requested copies of the software, including IBM, Hewlett-Packard, and most DOE National Laboratories. Use of SIMION allowed instrument designers at Hewlett-Packard to increase the sensitivity of a commercial mass spectrometer by an order of magnitude. Staff from INEL presented an invited course on the use of SIMION at the annual meeting of the American Society for Mass Spectrometry. Both the Plenary Session and the Instrumentation Session at that meeting features reports of

SIMION calculations. The impact of SIMION on modern mass spectrometry research and development was recognized by an R&D 100 award in 1989. The analytical chemistry effort at INEL is funded by the Division of Chemical Sciences.

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12. Supercritical Fluid Expansion Process Produces Uniform Particles for Thin Films and Fibers

Pacific Northwest Laboratory: R. D. Smith (CS)

A new method has been developed for the formation, directly from a vapor, of chemically and physically uniform submicron particles of many materials. The process is called Rapid Expansion of Supercritical Fluid Solutions (RESS) and uses supercritical fluids as solvents for the material to be deposited. The solution is rapidly expanded through a small nozzle from a supercritical fluid state into a volume where the solvent changes to a low pressure gas. The material thus released from solution forms fine particles that can be collected on a surface. The process lends itself to the formation of thin films and fibers and uniform mixtures of substances that cannot ordinarily be combined. Because many supercritical fluids form at room temperature, heat sensitive materials like biological molecules and organic polymers can be processed by this method. This work is a spin off from earlier research supported by Basic Energy Sciences and has been awarded several patents and an R&D 100 Award.

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13. Composite Optical/X-ray Laser Microscope

Princeton Plasma Physics Laboratory and Princeton X-Ray Laser: S. Suckewer (AEP)

The primary objective of the Composite Optical/X-Ray Laser Microscope (COXRALM) is to obtain images of biological cells revealing much finer detail than could be achieved with the use of an optical microscope. This so-called "high resolution" is possible due to operation at a wavelength much shorter than that used in optical microscopes. The light source used in COXRALM is a soft X-ray laser (SXL) producing short pulses of high intensity, well collimated radiation. It is expected that the COXRALM/SXL combination will enable the imaging of live cells.

COXRALM combines a high-contrast optical microscope for initial observation and manipulation of biological cells with a "contact" X-ray microscope. The biological cells are located directly on an optically transparent layer of material, called photoresist, which is sensitive to X-rays. After selection and initial observation with the optical microscope, the image of cells is created on photoresist with an SXL beam. In this procedure, the X-ray laser beam tube with a 0.1 micron thick silicon-nitride window on its tip (0.2mm x 0.2mm) is lowered until contact with cells is made. The photoresist is exposed by triggering the SXL. After development, a relief map of the X-ray

absorption by the specimen is formed on the surface of the photoresist. The photoresist is then coated with a thin layer of gold/palladium and viewed with a high-resolution scanning electron microscope.

COXRALM is unique because it allows a biologist to first choose and observe selected cells and then to obtain a high resolution image of these cells on photoresist.

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14. Micropol Polarimetric Detector for Liquid Chromatography
Ames Laboratory, Iowa State University: E. S. Yeung (CS)

Dr. Edward S. Yeung, Ames Laboratory, received the R&D 100 award in 1989 for his development of the "Micropol" polarimetric detector for liquid chromatography. This new laser-based polarimetric detector permits measurements on chiral molecules with minute rotations. The work previously received a technology transfer award from The Federal Laboratory Consortium.

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Small Business Innovation Research (SBIR) Accomplishments During FY 1989

Since its inception in 1983, DOE's Small Business Innovation Research (SBIR) program has been managed by the Office of Basic Energy Sciences. The program annually supports some 120 projects at a maximum level of \$50,000 for about six months. Around 50 of these "Phase I" projects are selected for further support under "Phase II" of the program for a maximum of two additional years with funding of up to \$500,000. Many of the small businesses that have received SBIR awards are showing success, both technical and commercial, and two important accomplishments resulting from DOE's SBIR program follow. Neither project falls within the Basic Energy Sciences Program areas, so the technical management of these programs was not performed under BES.

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15. Demonstration Project on Concentrated Solar Energy
ENTECH, Inc., Dallas, Texas: M. J. O'Neill (AEP)

Photovoltaic cells convert solar radiation directly to electricity; improving this process has generally been directed towards improving the efficiency of the photovoltaic cell material to carry out the conversion reaction. Under an SBIR project, a prismatic (Fresnel) lens system was developed and patented by ENTECH in which individual prism-like facets on the surface of a large rectangular area refract incident light, focusing it onto a narrow strip of solar cells below the lens system. On the underside of each strip of solar cells is a copper "heat-spreader" which reduces the operating temperature of the cells, increasing their efficiency. This unique, low cost concentrator, made of plastic, can be used with commercially-available photovoltaic cells.

Photovoltaic modules based on this concept have been designed, and an energy conversion efficiency of 17 percent, by far the highest commercial performance attained anywhere to date has been demonstrated.

The solar collector array tracks the sun, i.e., it is designed to maximize the radiation received. Two versions have been designed, the less complex (single axis system) achieving a solar concentration factor of 11.25, the more complex, full tracking (double axis) design achieving a concentration factor of 22.5. The SBIR funding of \$440,000 has been supplemented by an additional \$2,700,000 from the DOE photovoltaics program office and \$600,000 each from the 3M Corporation and the city of Austin, Texas. A 2,000 m², 300 kW DC demonstration plant is currently being built at the new 3M Office and Laboratory Center in Austin. The demonstration includes both the 11.25 and 22.5 versions of the patented Fresnel lens concentrator. In addition to working on the 3M demonstration plant, ENTECH has sold photovoltaic arrays and modules to Arizona Public Service Company and Pacific Gas and Electric Company of California.

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16. **Rapid Identification of Bacterium Based on Metabolism**
Biolog, Inc., Hayward, California: B. R. Bochner (AEP)

A technique has been developed to rapidly identify bacteria based on the chemical behavior of products of their metabolism. The technique makes a "breathprint" from the interaction of bacterial respiration products with preselected chemicals. Bacteria are exposed to 95 different selected chemicals; the digestion process for each bacterium is somewhat different making the "breath" an identifiable characteristic. The analyses are made possible by a versatile, automated patented chemical system.

Biolog, the developer of this technique, was cited in a Nature article that appeared on May 11, 1989, entitled, "Sleuthing out Bacterial Identities." The research leading to this technique was accomplished under a Phase I SBIR award that has been selected for continuation into Phase II. The technique employs a multi-trait analysis concept system with a patented color chemistry using dyes that react with products of the respiration process common to all bacteria. It determines simultaneously a bacterium's ability to digest 95 chemicals, producing a characteristic, analyzable "breathprint." A microplate, pre-coated with Biolog's patented chemistry, has 96 wells, each containing a different chemical food (carbon source) that may be taken up by the bacterium. Carbon source reactions result in color changes that are scanned automatically and interpreted by a computer.

Data of this kind are being used in DOE's Deep Subsurface Microbiology Program to characterize indigenous soil bacteria, and their capabilities for degrading pollutant molecules in the hope of using them for pollution clean-up. The technology also will find extensive applications in agro-business, food processing, genetic engineering, and medical technology.

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MATERIALS SCIENCES

1. Seeing the Glue that Holds Crystals Together

Lawrence Berkeley Laboratory: U. Dahmen, K. H. Westmacott, C. J. Hetherington and M. A. O'Keefe; Kyoto University: I. Yamada; University of Pennsylvania: V. Vitek; and Sandia National Laboratories/Livermore: M. J. Mills and M. S. Daw

Probing the mystery of how crystals are held together, scientists at LBL's National Center for Electron Microscopy (NCEM) have recently produced striking evidence for the precise arrangement of atoms at a crystal interface. Electron micrographs of unprecedented clarity, taken on the Atomic Resolution Microscope, have provided the first rigorous experimental test for two widely used theoretical grain boundary models. An exact match between the predicted and experimentally observed atomic structure for bicrystals of aluminum has been demonstrated. This breakthrough was made possible by combining in a collaborative network: thin film technology developed at Kyoto University; molecular statics calculations at the University of Pennsylvania and at Sandia National Laboratories in Livermore; and the unique high resolution capability of the Atomic Resolution Microscope (ARM) at Berkeley.

The prediction of the precise positions of atoms at interfaces, a goal of theoretical physicists for more than a decade, is now a reality. Geometrical models and systematic simulations by supercomputers have resulted in a framework for describing the structure as a function of misorientation in terms of structural units. Simulations are especially critical for aluminum which has an atypical crystal potential, and experimental tests for aluminum are particularly difficult because of the fine interatomic spacings in its close packed structure. To choose from more than a hundred possible input configurations for the computer simulations, scientists were guided by an elegant new technique for the direct determination of atomic displacements from electron micrographs. The technique, developed at the NCEM, allows the measurement of rigid body crystal displacements to an accuracy of better than 1/20 of an atom diameter. The resulting match between simulated interface structures and atomic resolution micrographs obtained with the ARM has validated the theoretical approaches and paved the way for the future exploration of the atomic behavior of grain boundaries.

The road is now clear for systematic studies of bicrystals in aluminum and other materials and will lead to new levels of understanding of strength, fracture and stability in polycrystalline materials. A number of as-yet untested theoretical predictions can now be put to test and, if verified, could lead to new advances in the science and technology of interfaces in a wide variety of materials.

* * * *

2. Molecular Oxygen on Cu(110): A Precursor to Oxidation
Oak Ridge National Laboratory: A. P. Baddorf and J. F. Wendelken

Molecular oxygen has been observed for the first time on the (110) surface of copper at a temperature of 15K. The oxygen molecules have been characterized using electron energy loss spectroscopy (EELS) and X-ray photoemission spectroscopy (XPS). As observed at higher sample temperatures, the first oxygen arriving at the surface dissociates, yielding atomic oxygen. After ~0.5 monolayer of atoms are produced on the surface, additional oxygen is adsorbed as molecules. Two molecular species were observed, one weakly bound to the surface with characteristics similar to gas phase oxygen, the other with vibrational and electronic levels characteristic of a chemical interaction with the copper. The O-O bond strength in this second species is 30% weaker than gaseous molecular oxygen phase. The weakly bound species desorbs at 35K. The chemically bound species dissociates at 50K and oxidizes the copper surface. These molecular species are radiation sensitive and exposures to X-rays or high energy electrons strongly promotes oxidation.

Understanding the copper oxidation is crucial for control of corrosion, obtaining minimal resistance at interfaces of electronic components, and in preparing novel high-temperature superconducting materials. In each case, gaseous diatomic oxygen dissociates into individual atoms on the surface. Thus the formation of a molecular oxygen species chemically bound to the surface, is an important intermediate step in the oxidation of copper. This work also reveals an exceptional reactivity of Cu(110) to small quantities of oxygen. Whereas copper was previously thought to react with molecular oxygen in a manner similar to silver, palladium or platinum surfaces, now Cu(110) should be classified with the more reactive surfaces of tungsten and chromium. This work also suggests a new procedure for producing very thin oxide films with low oxygen pressures.

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3. Novel, Low-Temperature Processes for the Growth and Oxidation of Silicon Nitride Thin Films
Sandia National Laboratories: J. W. Rogers, Jr., D. S. Blair, and C. H. F. Peden

Novel, low temperature processes have been developed for growing high quality silicon nitride (Si_3N_4) and silicon substrates. Silicon nitride is grown at 400-600°C using hydrazine (N_2H_4) as the nitriding gas instead of ammonia (NH_3) at ~ 900°C. The initial rates of nitridation are four times faster, and the nitride films are three times as thick when N_2H_4 is used. The silicon nitride films also were oxidized in a controlled manner using adsorbed potassium (K) as an oxidizing agent. The presence of K on the surface greatly lowers the temperature-time requirements (by over a factor of 100) for oxidation as compared with direct thermal oxidation of the nitride film.

Miniaturization in modern technology has created an increasing demand for stable very thin insulating films. Silicon nitride and oxynitride films,

widely used in the semiconductor and other industries for their passivating and/or dielectric properties, are considered an important key to further miniaturization. Current and/or potential applications include diffusion masks, surface passivation layers, nonvolatile semiconductor memories, and masks for selective oxidation. Direct thermal nitridation of the silicon by NH_3 at temperatures above 900°C is currently being examined as an alternate to the commonly used method in industry of chemical vapor deposition. However, high solid-state diffusion rates of silicon and nitrogen at 900°C cause degradation of the electrical properties and limit the minimum obtainable nitride layer thickness. Similarly, the high temperatures necessary to thermally oxidize the Si_3N_4 to form the oxynitride are not compatible with microelectronic processing and other advanced technologies. The processes developed in this work provide low-temperature synthetic routes for these important dielectrics which have the potential for overcoming current limitations.

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4. **New, Efficient Synthesis Route to Silicon Carbide** Ames Laboratory: T. J. Barton

A new, simple, efficient route to the synthesis of silicon carbide has been developed. In addition a process has been developed by which the silicon carbide adopts the highly-desirable, long-sought form of fibers. This process involves surface crosslinking of silylene-acetylene polymer fibers so as to allow maintenance of the fiber structure throughout the process of pyrolytic conversion to silicon carbide.

The industrial fabrication of silicon carbide fibers has been a technological secret closely guarded by the Japanese, and this result is a major breakthrough in this area. If this technology can be adapted to a continuous process, it has the distinct possibility of cutting both the time and cost of current commercial routes to SiC fibers. SiC fibers are used in composites which are displacing metals in industrial applications due to their high strength, low weight, high heat tolerance, and resistance to chemical breakdown.

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5. **Calculations of the Heat of Formation of Alloys** Brookhaven National Laboratory: R. E. Watson, M. Weinert, J. W. Davenport, and G. W. Fernando

One of the most important quantities in materials science is the energy or heat released when two metals are combined to form an alloy. The heat released is an indication of bond strength. Many of the best materials for strength or high temperature properties are alloys rather than pure materials. Yet the number of possible combinations is so large that theoretical guidance can be enormously helpful in choosing promising new alloys.

In recent years it has become possible to calculate these heats from first principles using a theory, the local density approximation, which contains no adjustable parameters and therefore is not biased by the expected outcome.

This theory has recently been applied to a series of 24 alloys typified by titanium-platinum. The calculations successfully predicted the crystal structure for 50/50 alloys and for other compositions as well as the high heats of formation found experimentally. The underlying reason for strong bonds can be seen in the properties of the electronic density of states. Calculations of this type are not limited to the metals studied here. Unknown alloy properties can be easily predicted. In recent work, the technologically important material nickel aluminum has been investigated.

Calculations of this type are expected to be extremely helpful in searching for new alloy combinations.

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6. Direct Atomic View of the Oxidation of Silicon (Si) Surfaces University of Illinois: T. C. Chiang

The oxidation of silicon surfaces is an important step in the fabrication of microelectronic devices. Using a scanning tunneling microscope, the oxidation processes occurring on the Si(111) surface were observed for the first time with atomic resolution in real time. A given area on the surface is continually scanned and viewed by the microscope, while the oxidation takes place in an ultra high vacuum chamber. The results show that individual atomic defects commonly found on this surface after prolonged heat treatment act as nucleation centers around which the oxidation initiates and expands. The resulting surface is disordered. An interesting observation is that atomic steps commonly found on this surface are insensitive to oxygen exposure as are atomically flat areas on the surface. This shows that the atomic steps are stabilized by the reconstruction.

A detailed understanding of the oxidation of silicon is crucial for the improvements for the processing and fabrication of microelectronic devices. The roles played by surface defects and atomic steps in the oxidation process need to be clarified for a full control for the device structure and the resulting electronic properties.

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7. "Sugar-Coated" Semiconductor Surfaces Lawrence Berkeley Laboratory: M. Bednarski, L. Oehler, and M. Mastandrea

One important potential role for enzymes in materials synthesis is the modification of surfaces to alter and control interfacial properties. Scientists at the Center for Advanced Materials at Lawrence Berkeley Laboratory have devised a chemo-enzymatic process that allows them to coat the surface of doped silicon wafers with specifically designed carbohydrates. In addition to altered physical properties, these modified materials exhibit

dramatic and controllable alterations in specific and nonspecific adhesion. Gram-negative bacteria binds easily to the unmodified silicon wafer. Enzymatic attachment of the sugars, mannose or galactose, is then possible because the surface bound bacteria have specific receptors for these sugars but no receptors for glucose, a structurally quite similar sugar. Surface modifications of this sort have potential in a number of areas. Attachment of recognition sites to semiconductor surfaces should allow the development of selective sensors. Attachment of hydrophilic or hydrophobic groups should allow control of the lubricative or adhesive nature of the surface. Attachment of amino acids with reactive groups such as thiols should allow selective, uniform, and dense binding of films of materials such as gold.

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8. New Ion Conducting Polymers

Brookhaven National Laboratory: T. Skotheim; and Polytechnic University: T. Okamoto

A new class of ion conducting polymers with the highest room temperature conductivity ever measured for such materials has been developed. Room temperature conductivity for lithium ions has been measured at 25°C and found to be higher by a factor of 10 than for any other polymeric material. The polymer electrolytes are based on polysiloxane backbones with polyether side chains. It is anticipated that this development will have an important impact on the development of a number of thin film electrochemical energy technologies, in particular thin film rechargeable lithium batteries and electrochromic windows.

Thin film rechargeable lithium batteries based on polymer solid electrolytes, lithium anodes, and lithium intercalation materials used as cathodes have theoretical energy storage capacities more than 10 times that of lead-acid or nickel-cadmium batteries. This class of materials is particularly attractive for long term energy storage because self-discharge is virtually absent. Self-discharge rates for lithium batteries has been reported at values less than 0.1 percent per year, implying a shelf-life of more than 10 years.

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9. New Technique Provides Surface Atom Detection

Sandia National Laboratories/Livermore: M. Lapp, R. J. Anderson and J. C. Hamilton

Minute amounts of molecules on technologically-important surfaces can now be detected as a result of recent advances in optical measurement techniques. The measurements can be made in chambers which can be operated at pressures ranging from ultra-high vacuum to atmospheric pressure. Most recently, the new method was used to probe the surface of palladium, leading to the discovery of a dramatic observable effect from hydrogen adsorbed on the surface. This resonance behavior was not observed for carbon monoxide adsorption. The hydrogen adsorption effect has been explained in terms of the surface electronic structure of palladium being changed by the hydrogen.

This discovery is important for both fundamental and applied reasons:

1) Scientifically, the dramatic effect observed for a system with well understood surface electronic structure will allow theoretical calculations of second harmonic generation leading to a better understanding of these phenomena.

2) The observed effect will greatly facilitate the study of the interaction of hydrogen and its isotopes with palladium. Such phenomena play a major role in hydrogen storage, catalysis, surface diffusion and other technologically important processes. The observation opens up the possibility of dynamic studies with species-selective detection at atmospheric pressures.

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10. Development of a Low-Temperature Sinterable Lanthanum Chromite
University of Missouri at Rolla: H. U. Anderson, S. A. Howard, D. M. Sparlin

Through the careful control of selected dopants, lanthanum chromite, an important component material in Solid Oxide Fuel Cells and other applications, can now be sintered in air to high density at temperatures of 1400°C and below without compromising the high electrical conductivity or high-temperature stability of this material under fuel cell conditions. This was accomplished by the partial substitution of calcium for lanthanum and cobalt for chromium in the lanthanum chromite system. Sinterability of this material at low temperatures is necessary to be compatible with the sintering characteristics of other fuel cell component materials.

These results will allow Solid Oxide Fuel Cell researchers and manufacturers to process fuel cells with lanthanum chromite as the interconnect material under conditions that are compatible with other fuel cell components. This will eliminate one of the major obstacles to utilization of Solid Oxide Fuel Cells (processing economics) and should accelerate the commercialization of Solid Oxide Fuel Cells.

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11. Silicon Epitaxial Growth Dilemma Solved
Sandia National Laboratories/Albuquerque: E. Chason and J. Y. Tsao

A new atomistic model of a growing silicon crystal surface during molecular beam epitaxy (MBE) has been developed at Sandia National Laboratories. This model is found to explain the dilemma of how smooth growth is maintained even at temperatures so low that lattice matching (epitaxy) proceeds by cyclical nucleation and coalescence of islands. In this model, growth proceeds by strings of atoms which result from the surface reconstruction of the silicon surface atoms. These strings grow directionally, with the growth direction rotating 90° on each subsequent layer of atoms. Topologically, missing strings must be filled in before the perpendicular growth of a string on the next layer can continue. This constraint provides a mechanism by which

silicon can maintain smooth growth. This model provides an understanding of previously unexplained and surprising observations of persistent RHEED oscillations under certain conditions of silicon molecular beam epitaxy. Moreover, recent scanning tunneling microscopy studies of the silicon surface after growth have confirmed the existence of these hypothesized strings and the string blocking mechanism.

Understanding the mechanisms which lead to the epitaxial growth of very smooth surfaces is of crucial importance to advanced microelectronic and optoelectronic concepts. While surface reconstruction has long been believed to play an important role in lattice matched (epitaxial) growth, this is the first time such a direct role has been demonstrated. Moreover, this key conceptual advance provides a foundation for future progress. It is anticipated that detailed examination of string interactions with surface steps will allow a fully atomistic picture of silicon molecular beam epitaxial growth based on strings to be developed. Such advances provide a basis for better control of thin layer growth of the very important electronic material, silicon, and perhaps also may lead to progress in the growth of compound semiconductors used for optoelectronic devices. These advanced device concepts depend almost exclusively on layered materials with extremely sharp interfaces. While the static structure of surfaces is well-studied, very little is known about the nature of the dynamic surface during lattice matched (epitaxial) growth. For example, even for the best studied case of silicon, the fundamental defects controlling lattice matching were not previously known. Yet an ability to control the surface smoothness and produce increasingly sharp interfaces and thin layers will be of key importance to future advances in microelectronics.

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12. Structure of Boron Carbide Thermoelectrics

Sandia National Laboratories: T. L. Aselage, D. Emin and D. R. Tallant

Although the arrangements of atoms within crystalline solids are usually ordered, how and why boron carbide crystals are substitutionally disordered has been established. The new theory predicts where boron and carbon substitute for one another within the boron carbide crystalline framework. Measurements of the vibrations of the solid's atoms against one another confirm the arrangements of atoms predicted. Changing the arrangement of boron and carbon atoms within boron carbides can significantly affect the flows of heat and electronic charges through the boron carbides. In particular, by changing the ratio of boron and carbon atoms boron carbides are converted from crystal-like thermal conductors to glass-like thermal insulators.

Boron carbides show promise for use in the direct conversion of heat to electricity at very high temperatures. By operating at very high temperature, boron carbide thermoelectric generators have potential for much higher conversion efficiency than conventional systems. Thermoelectric power generation requires the combination of segments in which the charge carriers are negatively charged (n-type) with segments in which the charge carriers are positively charged (p-type). Very efficient high-temperature p-type

thermoelectrics already have been produced. The theory developed and confirmed indicates that the addition of a sufficient quantity of an appropriate third element will result in an n-type boron carbide. With an efficient n-type boron carbide as a complement to the already efficient p-type boron carbide, the first all boron carbide thermoelectric generator would have been produced. Basing a thermoelectric device on a single material simplifies the design and enhances the long-term high-temperature stability.

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13. Oriented Ceramic Crystal Growth Utilizing Biological Processes
Pacific Northwest Laboratory: P. C. Rieke and B. J. Tarasevich

A new method for growing oriented ceramic thin films has been developed. This technique involves mimicking biological processes utilized in the natural growth of seashells, bone, tooth enamel, etc., to grow oriented thin films of a desired ceramic material. This process is unique in that it uses a surface-modified polymer as a template to control crystal orientation and size as the crystals grow from a solution. Crystal growth occurs only where the polymer has been modified; therefore, patterning is easily achieved by selective polymer surface modification. The process is conducted at near room temperature and essentially controls the placement and orientation of each ceramic crystal. Oriented films as thin as 200 Å and as thick as several microns have been grown. This process offers a method of combining polymers and ceramics into unique monolithic composite materials which have high resistance to brittle failure. Understanding the processes utilized by nature will allow composite materials with more desirable properties, e.g., inorganic polymers and stronger ceramics to be combined. An entirely new class of ceramic matrix composite materials can now be fabricated, containing only a few percent polymer in layered form, that controls crystal orientation and greatly influences fracture toughness of the material.

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14. Experimental Determination and Calculation of the Atomic Structure of Grain Boundaries in Metals
Massachusetts Institute of Technology: I. Majid, P. D. Bristowe, and R. W. Balluffi

The first successful agreement has been obtained between calculated and experimentally determined atomic structures for a systematic series of grain boundaries. The atomic structures of a series of different grain boundaries in gold were recently calculated by means of computer simulation using the Embedded Atom Model. Subsequent X-ray diffraction structure analysis demonstrated experimentally that the computed structures are essentially correct. The model has the advantage that it is reasonably simple and can be used to calculate the equilibrium configuration of grain boundary systems containing large numbers of atoms by computer simulation.

boundary structure factors which markedly increases the ability to determine boundary structure.

The calculated boundary structures using the Embedded Atom Model were highly consistent with measured X-ray structure factors for these same boundaries. Systems containing large numbers of atoms can be handled in computer simulations using the Embedded Atom Model, and, now, the way seems to be open to the more reliable calculation of important large scale grain boundary kinetic phenomena such as grain boundary diffusion and migration and, also, mechanical property phenomena.

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15. Grain Boundary Disorder: A Key to the Ductility of Ordered Alloys
Dartmouth College: E. M. Schulson and I. Baker

Recent research has revealed that the addition of boron to alloys of Ni_3Al on the Ni-rich side of the compound imparts extensive ductility to an otherwise brittle material. The important implication of this research is that the ductility of both Ni_3Al and Ni_3Si relate directly to the ease with which slip is either accommodated or transmitted at grain boundaries, which, in turn, is related to the degree of grain boundary disorder.

Experimental studies have revealed that grain boundaries in the strongly-ordered intermetallic compound Ni_3Al become highly enriched in Ni and depleted in Al (relative to the matrix) when boron is added to alloys on the Ni-rich side of the compound. Also, the addition of boron lowers the effectiveness with which grain boundaries impede slip. When boron is added to alloys on the Al side of stoichiometry, the alloys remain brittle and no change is seen in the grain boundary impediment to slip. Effects similar to these have been noted in the isostructural alloy Ni_3Si .

One of the promising avenues for raising the operating temperatures of turbines is to employ intermetallic alloys as a means of improving the high temperature stability of the compounds. An implication of these results is that a requirement for tensile ductility of strongly ordered alloys susceptible to brittle intergranular fracture, in addition to sufficient independent deformation modes, is that the grain boundary region be at least partially disordered. This program has provided one of the potential avenues for achieving ductility in otherwise brittle materials.

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16. Critical Currents and Grain Boundary Dislocations in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ Superconductors
Oak Ridge National Laboratory: M. F. Chisholm and S. J. Pennycook

A new electron microscopy method for forming high-resolution images with strong chemical sensitivity has been used to examine grain boundaries in the

* See footnote on page 4

high-temperature oxide superconductors. The new method forms images using large-angle elastically scattered electrons. Thus, the image is not a reconstruction of the object from the diffracted beams, as in phase contrast, but instead a map showing at atomic resolution the scattering power of the sample. The scattering power for high-angle scattering is strongly dependent on atomic number Z , giving the images chemical sensitivity. Using this technique, for the first time the true nature of the defects present at individual low-angle tilt grain boundaries that are responsible for the drastic reduction in the critical current density in this material has been shown. Such boundaries are seen to consist of an asymmetric array of dislocations. When the boundary tilt angle exceeds -7.5° , the defects are amorphous and chemically identical to the adjacent $\text{YBa}_2\text{Cu}_3\text{O}_{6-x}$ grains.

This research demonstrates that the achievement of high critical current densities in the oxide superconductors depends strongly on the boundary geometry. Segregation of impurities or the formation of intergranular glassy phases is not necessary to produce drastic reductions in critical currents. The disturbed region associated with the defects that are obstacles to current flow is the result of intrinsic structural relaxation of a chemically clean boundary. As the tilt angle increases, the number of defects increases further, restricting the superconducting path. This kind of information is needed for unraveling the most important problem of critical currents in the ceramic superconductors; also, it illustrates the usefulness of the high-resolution chemical sensitivity of Z -contrast imaging.

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17. **Electrical Transport in Transition-Metal Carbides**
Oak Ridge National Laboratory: F. A. Modine; and Oklahoma State University: C. Y. Allison

Many studies of electrical transport in the transition-metal carbides have been made, but reproducible results and a theoretical understanding of the observed effects have been elusive because well-characterized single crystals have not been readily available and careful measurements have rarely been made. Recent systematic studies of several transition-metal carbides, however, provide some convincing connections with theory. The electrical properties of transition-metal carbides appear similar to those of transition-metal alloys. The temperature dependence of the electrical resistivities is described by one or the other of two well-established theories.

A new theoretical description of electrical transport in the transition-metal carbides has emerged. Moreover, connections between superconducting and normal state properties can be based upon the similar electron phonon interactions that are involved under either superconducting or normal conditions. Furthermore, low-temperature phenomena provide a simple measure of the carbon content of a transition-metal carbide crystal, which is the single most important characterization factor for these materials.

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18. Lattice Stiffening Observed During Superconducting Transition
Argonne National Laboratory: L. Rehn, R. Sharma, P. Baldo, and J. Liu

The first direct evidence of an abrupt stiffening of the crystal lattice at the superconducting transition temperature has been obtained using the unique technique of ion channeling. The measurements, performed on highly perfect single crystals of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$, involve steering an ion beam along the channels between atomic rows and planes of the single crystal. The scattering of the individual ions within the channels provides a direct probe of the vibrational amplitudes and, hence, lattice stiffness. The results show a faster than normal increase in lattice stiffness (decrease in vibrational amplitude) as the temperature is decreased, corresponding to a significant increase in the Debye temperature, and the first direct evidence of a step-wise increase in lattice stiffness at the superconducting transition temperature. Indirect evidence provided by the interpretation of neutron diffraction data has also shown lattice stiffening upon cooling but only hinted at the abrupt change at the transition temperature, which has now been clearly demonstrated by ion channeling. Structural information, also obtained by the channeling technique, confirms that no crystallographic transformation occurs at the transition temperature.

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19. High- T_c Superconducting Bolometer
Lawrence Berkeley Laboratory: P. Richards and S. Verghese; and Stanford University: T. Geballe and S. Spielman

Detailed theoretical analyses coupled with confirming experimental measurements have shown that a bolometric infrared detector with very useful properties can be made using the resistive transition of a high- T_c superconducting film as the thermometer. Unlike many applications discussed for high- T_c materials, this high- T_c bolometer can be made with presently available films. The effect of noise mechanisms that limit sensitivity of infrared detectors can generally be reduced by the use of low operating temperatures. For wavelengths shorter than $20 \times 10^{-6} \text{m}$, liquid-nitrogen-temperature photovoltaic detectors are widely used and are very sensitive. At longer wavelengths, however, no satisfactory cooled detector technology has been available heretofore above liquid-helium temperatures. This collaborative research has shown that a liquid nitrogen cooled high- T_c bolometer can be used for wavelengths longer than $20 \times 10^{-6} \text{m}$. Possible near-future applications for this new technology include detectors for laboratory spectrometers and for observations of the earth from passively cooled spacecraft.

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20. High Temperature Superconductors
Sandia National Laboratories/Livermore: R. J. Anderson and J. C. Hamilton

Important new insights have been gained for yttrium-based and thallium-based superconductors concerning their fundamental properties and the relationship between these properties and processing conditions. Processing studies of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ used in situ Raman spectroscopy to determine the relationship between

oxygen defects, temperature, and superconducting transition temperature. A phase transition involving the disordering of oxygen within the structure was observed for the first time. Furthermore, a particular lattice vibrational mode was found to give a direct measure of the density of oxygen defects in the structure. In a collaborative study, the technique of substituting oxygen at selective sites in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ was demonstrated by using Raman analysis to determine the distribution of oxygen isotopes at different sites within the structure. Fundamental characterization of the Raman-active phonons of four different thallium-based superconductors were performed by polarization studies of oriented single crystals. This information was then used to characterize the spatial distribution of phases within polycrystals. By Raman microscopy, it was found that the majority of thallium-based crystals had intergrowths of several phases within them.

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21. Observation of Phonon Coupling in a High T_c Superconductor
Argonne National Laboratory: D. G. Hinks, D. R. Richards, and B. Dabrowski

Careful measurements on the $\text{Ba}_x\text{K}_{1-x}\text{BiO}_3$ system which has a superconducting transition temperature (T_c) of 30K has permitted the unequivocal determination of an isotope effect on T_c , thus showing a major role for electron-lattice vibration interactions in a high temperature superconductor. This work has been possible because of the development of a unique, highly simplified method for the synthesis of the compounds. With good samples available, a large number of pertinent basic properties, including structural phase relationships, normal-state resistivity, superconducting energy gap and critical fields have been measured. As a result, this is one of the most completely characterized oxide superconductors currently available.

The recognition of the important role of phonon coupling in this system will allow the development of realistic models that can be used to help predict the additional technologically important properties of the system, namely critical field and ultimate critical current. Since the structure of this superconductor is cubic, it will be easier to theoretically model its properties in a realistic manner than is possible for the highly anisotropic high temperature superconductors that contain copper. It should also be possible to use these results to evaluate the role of phonon coupling in other compounds, and so achieve better understanding of the ultimate T_c in the oxide superconductors generally.

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22. KTaO_3 - A New Substrate Material for High- T_c Superconducting Films
Oak Ridge National Laboratory: R. Feenstra and L. A. Boatner

A new crystalline substrate for the formation of epitaxial thin films of high- T_c superconductors has been discovered. The new material, potassium tantalate or KTaO_3 , can be used to grow thin, aligned crystalline films of the $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ family of high-temperature superconductors. Substrate materials for the epitaxial growth of thin films must meet a set of stringent requirements

including a close match between the lattice constants of the film and substrate and a high degree of chemical inertness to prevent film-substrate reactions that destroy the superconducting properties of the film. The new materials meet both of these critical criteria. In fact, the $\text{KTaO}_3/\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ system is apparently characterized by a lower degree of film/substrate interaction than that associated with any previously employed substrate material such as SrTiO_3 . Fortunately, the new substrate material can be grown in the form of large single crystals by means of a simple technique so that it is a practical material for the production of large-scale electronic devices.

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CHEMICAL SCIENCES

23. **Observed Energy Transfer Process Not Considered in Theories**
Brookhaven National Laboratory: R. Weston and T. Sears; Columbia University: G. Flynn

At high temperatures typical of combustion systems, unimolecular reactions are quite important. In such reactions, the transfer of vibrational energy between highly excited reactant molecules and molecules at ambient temperature plays a very important role in the reaction process. The molecules at ambient temperature greatly outnumber the excited ones and are referred to as "bath" molecules. Presently existing theories of energy transfer from highly excited molecules do not provide information about the final state of the "bath" molecule and, in general, tend to omit possible excitation in the bath species. In recent work, using diode laser technology to monitor CO_2 "bath" molecules, it was observed that as much as 25% of the initial energy in the excited reactant molecules is converted by collision to vibrational energy in CO_2 and that the populations of the various product vibrations is in disagreement even with a statistical model. Clearly, more development is needed to enable accurate phenomenological prediction of unimolecular processes.

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24. **New Spectroscopic Technique for Testing Theories of Molecular Rearrangements**
Massachusetts Institute of Technology: R. Field

A new spectroscopic technique had been demonstrated that can provide unique information on the properties of highly energetic molecules found in combustion environments and will allow critical tests of chemical reaction theories. Called stimulated emission pumping (SEP), the technique permits researchers to relate complex spectra to the underlying potential energy function driving chemical reactions. Spectroscopy has traditionally provided information on the potential energy functions of molecules but only for stable species at low temperatures far from the energetic conditions characteristic of chemical reactions where spectra are orderly and easily interpreted. At higher temperatures, spectra become extraordinarily complex to the point that many believed the spectra of molecules approaching chemical reactions would be uninterpretable. Using SEP, the high temperature isomerization of the vinylidene radical, H_2CC , to acetylene, HCCH ; a typical intramolecular H-atom

migration has been characterized. Theoreticians have been able to calculate a potential energy function for this isomerization. A critical feature of the untested theory was the existence of an energy barrier to the isomerization. The SEP approach has now confirmed the existence of the predicted energy barrier and has provided an upper bound for the conversion of vinylidene to acetylene. The technique may provide a powerful and general scheme for detecting isomerization processes involving H-atom migration and exchange.

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25. Colloidal Semiconductor Particles of Predetermined Size Produced by Pulsed Radiolysis

Argonne National Laboratory: D. Meisel

Semiconductor particles dispersed in solution as colloids can be grown to predetermined size specifications. Prompted by a discovery at Bell Laboratories that electronic and photocatalytic properties of semiconductors are altered at very small sizes (5-50 Å or 50-500 billionths of a centimeter), radiation chemists have developed a method for growing tiny semiconductor particles of uniform size. Crystallization is initiated by a pulsed electron beam from a linear accelerator. Cadmium sulfide, for example, is prepared by electron attachment to organosulfide molecules, releasing sulfide ions into solution which react with cadmium ions. Because the electron beam is nearly instantaneous and generates a homogeneous distribution of reactants, the resulting particles possess a narrow size distribution. The size is controlled by the concentration ratio of the reactants, or by added inert, complexing ions. Spectroscopic studies of the colloidal solutions at various stages of growth, from isolated molecules through agglomeration of small clusters, indicate that cadmium sulfide particles begin to exhibit the electronic and crystalline properties of the bulk material when the diameter reaches 15±2 Å.

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26. Evidence Found for New Atomic Collision Process

Oak Ridge National Laboratory: S. Datz

Scientists have obtained the first experimental evidence for a new atomic collision process leading to production of radiation. The new results show that an ion can be excited during a collision, not because of its interaction with the electron that is captured as in Resonance Transfer with Excitation (RTE) or in Dielectronic Recombination (DR), but with a second uncaptured electron that remains on the target atom after the ion-atom collision. The new interaction is labeled 2eTE. In DR an electron in an atomic ion is excited simultaneously while capturing a free unbound electron. In RTE the same excitation occurs but the ion captures the bound electron from a neutral atom upon collision. In all three processes, DR, RTE and 2eTE, capture and excitation takes place simultaneously. It is a correlated process, i.e., one step is synchronous with the other, leading to a resonant process. In all three processes, DR, RTE and now 2eTE, the excitation is prompted by an electron-electron interaction where two electrons, one from each of the collision partners, interact with one another. Documenting these processes is important to fusion energy development since the emission of radiation is an undesirable energy loss process in fusion

oriented plasmas. These excitation processes are among the least documented fundamental interactions in atomic physics. The discovery of a new excitation channel in a seemingly simple process indicates the importance of continuing research in this area.

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27. New Spectroscopic Technique Applied to Free Radicals
University of Pennsylvania: H. L. Dai

Stimulated Emission Pumping (SEP) an optical, double-resonance spectroscopy technique is proving to be a powerful method for studying the properties of elusive chemical species characteristic of combustion systems. In the SEP experiment, the energy separation between two states is accessed by pumping species from the first state to a third state, much higher in energy, and then stimulating emission from the third state back down to the second state. These pump-probe measurements require two lasers tuned in resonance to the two energy level separations. The technique is highly specific and sensitive compared with single-resonance spectroscopic techniques, but the specificity and sensitivity are achieved at the cost of experimental complexity. Now SEP has been used to study the time dependence of the transient free radical CH_2 where the experimental challenge has been the very low concentration of the radical. CH_2 is an important intermediate in combustion and is prepared in the laboratory by laser photolysis of $\text{H}_2\text{C}=\text{C}=\text{O}$. Under the experimental conditions used, the lifetime of the CH_2 radical is on the order of 100 nanoseconds (.0000001s). Even with this short lifetime and at low concentrations, strong spectral signals were observed and assigned. The strength of the signals, coupled with the short time scale for performing the measurement will allow SEP to be used to study the reaction kinetics of CH_2 as a function of internal energy.

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28. Reaction Rate Data Confirm the Role of Quantum Mechanical Tunneling in Chemical Reactions
Argonne National Laboratory: A. Wagner; University of Illinois at Chicago: R. Gorden

Scientists at Argonne National Laboratory and the University of Illinois at Chicago in separate but complementary studies have confirmed the role of hydrogen molecules to yield the chemical radical OH and a hydrogen atom as products. The effect of quantum mechanical tunneling is to allow chemical reactions to take place when the combined energy of the reacting species is insufficient to break the chemical bonds of the reactants, in this case the H_2 bond. Knowledge of the influence of tunneling is necessary to extrapolate chemical reaction rates from temperatures and pressures characteristic of laboratory measurements to conditions characteristic of combustion processes. Because hydrogen is the lightest element, it is expected to exhibit the largest quantum mechanical tunneling effect. Earlier measurements of $\text{H}_2 + \text{O}$ and $\text{HD} + \text{O}$ reported last year had indicated that tunneling might indeed have a significant influence on the temperature dependence of the reaction rate. The recent measurements of $\text{D}_2 + \text{O}$ now confirm the earlier measurements. The data have been compared with theoretical predictions from Argonne, the University of Minnesota

and Emory University, all of which were supported by the DOE Office of Basic Energy Sciences. Agreement between both sets of measurements and both theoretical calculations was excellent. The theory and data will be useful in placing limits on the influence of tunneling in other chemical reactions.

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29. Spectral Hole Burning: a New Window on Photosynthesis
Ames Laboratory: J. Small

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

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30. Surprising Molecular Rearrangement Seen in Molecular Beam Studies
Lawrence Berkeley Laboratory: Y. Lee

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

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31. Laser Techniques May Improve Age-Dating Capabilities
Pacific Northwest Laboratory: T. Whitaker

Researchers at the Pacific Northwest Laboratory are developing laser-based techniques for dating materials by measuring rare noble gas isotopes. High-resolution, continuous-wave resonance ionization mass spectroscopy improves the sensitivity of traditional mass spectrometry through more efficient ionization. In addition, isotope-specific laser excitation makes it 1,000 to one million times more selective than conventional ion sources. Isotope ratio measurements for various noble gas isotopes can be used to date samples such as ground water from five to one million years old. Such ground-water dating can be used to help characterize existing or potential waste disposal sites for chemical or long-lived radioactive waste.

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32. New Capability in the Detection and Characterization of Actinides in Aqueous Solution
Argonne National Laboratory: J. Beitz

The difficult detection and characterization of the actinides uranium, neptunium, plutonium, and americium in aqueous solution have been advanced to a new high level of sensitivity by chemists at Argonne National Laboratory. The technique, called laser photoacoustic spectroscopy, LPAS, monitors the acoustic wave that results from the tiny burst of heat generated by the absorption of the laser beam by the actinide species. This is a difficult determination because of the expected low solubility of the actinide-containing material. These actinides can now be analyzed to concentrations as low as about one microgram in a liter of solution which represents a three-fold increase in sensitivity over that previously possible for these elements. In addition, this can be achieved in a variety of types of solutions ranging from acid to alkaline and over a broad temperature range including ground waters which are at elevated temperatures typical of those found around a nuclear waste repository. Spurious signals are obtained from suspended particles and colloids which can scatter the laser light. Research is under way to minimize this problem without changing the chemistry of the solution under study. Capabilities such as these will provide the necessary expertise and techniques for the characterization of nuclear waste repositories in licensing procedures. This effort recently received the ANL Pacesetter Award for technical excellence.

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33. Efficient Fusion Observed in Molecular Cluster Collisions
Brookhaven National Laboratory: L. Friedman, R. J. Beuhler, and G. Friedlander

Scientists from Brookhaven National Laboratory have observed deuteron-deuteron fusion reactions resulting from collisions of singly charged clusters of deuterium oxide (D_2O), accelerated to 200 to 325 keV, with titanium deuteride surfaces. Fusion was identified primarily by the detection of 3.0 MeV protons resulting from the reaction ${}^2H+{}^2H \rightarrow {}^1H+{}^3H$. The fusion reaction rate, as measured by the counting rate of the emitted protons, is found to increase

linearly with the kinetic energy of the cluster. The fusion reaction rate exhibits a broad maximum around 200 molecules of D_2O per cluster. The reaction rate is somewhat more than 10 orders of magnitude greater than expected from the reaction cross section for single collisions of 300 eV deuterons (the average kinetic energy per deuteron in the cluster). Although no detailed model for the process has yet been proposed, the Brookhaven scientists believe that the enhanced reaction rate is a direct consequence of the relatively long confinement time of approximately 10^{-13} seconds resulting from the penetration of the cluster into the target.

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ENGINEERING AND GEOSCIENCES

34. Thinning and Rupture of Thin Liquid Films Northwestern University: S. G. Bankoff and S. H. Davis (EG/E)

In many heat transfer situations, it is important that the heat transfer surfaces are covered continuously with liquids; the role of the liquid is to enhance the rate of heat transfer and control the temperature of the surface. Examples of devices in which thin liquid films play an important role are boiler tubes, steam generators, heat pipes, belt and filament radiators for heat rejection in space, and microchips in supercomputers.

Draining of the liquid film or increasing heat flow, or both, may thin out the liquid film and ultimately rupture it, resulting in a dry spot. The disruption of heat transfer at the dry spot will cause the local surface temperature to increase dramatically and in many cases will lead to a failure of the equipment. Thus, enormous efforts have been directed at understanding, predicting and ultimately precluding the occurrence of dry spots in heat transfer equipment and apparatus.

In the present project, a theory for describing the evolution of a thin liquid film on both horizontal and tilted planes heated uniformly and nonuniformly has been developed and confirmed experimentally. The theoretical description divides the process of thinning and rupture into two stages. In the first stage, the film thins out due to evaporation and/or draining. The second stage involves a further decrease in thickness and eventual rupture of the locally very thin film ($\ll 1$ micron thick). At this stage the processes are governed by the details of molecular interactions. This in turn is modified by forces acting on the film surface due to minute nonuniformities in the surface temperature, the so-called thermocapillary forces.

Now that the details of the onset of dry spots are better understood, it may be possible to mitigate the physical factors leading to this onset. Thus this new capability of predicting the dry out phenomenon will allow future designers to optimize the performance of various kinds of heat exchangers.

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35. Intelligent Machines in Unstructured Environment
Oak Ridge National Laboratory: C. Weisbin (EG/E)

A challenging task in the context of environmental restoration is the protection of humans in the process of cleaning up toxic spills, and transportation and storage of high activity nuclear wastes. Ideally what is needed is a system acting autonomously under loose remote human supervision. Autonomy and the limitation to loose supervision imply a certain degree of intelligence. The technical infrastructure for the desired degree of intelligence is the subject of research at the Center for Engineering Systems Advanced Research (CESAR) at ORNL.

A test bed for exploring various approaches to this problem is a small mobile robot, HERMIES-IIB. In a recent demonstration, HERMIES was given the task of starting from a given location, determining the path through an obstacle strewn floor to an instrument panel, on arrival at the panel reading its instruments, and, if need be, manipulating some controls so as to obtain a prescribed instrument reading. The status of the instrument readings and the required sequence of manipulations were not known by HERMIES at the outset of the experiment.

Successful completion of this task required that HERMIES build a world model from sparse and inexact sensory data (sound & sight), choose appropriate navigation paths to reach the destination as soon as possible, deal gracefully with unexpected events (eg. moving obstacles), sequence strategy based upon previous "similar" (but not identical) experience, and implement the strategy using vision-guided manipulation. At the heart of the robot's intelligence is a real-time expert system dealing with numerical and symbolic information forming a basis for decision making in the presence of unexpected events. It is a "natural" way to extend smoothly the competence of the robot, and to explain on demand its actions to the supervisor. Currently the system is capable of considering several different unexpected events at the same time.

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36. A New More Efficient Energy Conversion System
Stanford University: J. Ross (EG/E)

In nature the conversion of chemical energy to mechanical energy for instance through burning a fuel to generate heat, appears to be more efficient than what can be achieved by conventional means in man-made systems. A possible reason is that, in a man-made system such as a steam turbine, the fuel is delivered to the engine at a steady rate, while in nature, the process is time dependent. For instance, the conversion of the energy in glucose to muscle power, a very efficient process, shows a well defined characteristic oscillation. Past analysis of those oscillations showed that their presence introduces a control parameter which nature can be uses to minimize losses in this biochemical energy conversion system.

Taking a cue from this observation Professor John Ross has shown that the efficiency of a thermal engine can be enhanced significantly by modulating the rate at which the fuel is fed to the engine. Theoretical results were

confirmed in a preliminary experiment in which the feed rate of the fuel was turned up and down periodically. That resulted in corresponding large variations of the temperature of the exhaust gas, with the peak temperature far exceeding that expected in steady burning of the fuel. This higher temperature alone would lead to a more efficient operation of the engine. But in addition, advantage is taken of the change of the flow pattern in the hot gas, resulting in reduced heat losses through thermal conduction.

While the increase in efficiency expected from this experiment was about 2% over steady state operation of the combustor, theoretical considerations show that as much as a 40% increase in efficiency is possible. A patent for this energy conversion process has been issued.

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37. Deep Drilling Project Sheds New Light on Volcanoes Los Alamos National Laboratory: J. Gardner (EG/G)

Calderas are collapsed craters resulting from the largest, most explosive volcanic eruptions documented in the Earth's geologic record, and they are the surface representation of large volumes of magma (or molten rock) accumulated at relatively shallow depths in the crust. The vast heat content and high subsurface temperatures associated with shallow, crystallizing magma create dynamic systems of hot groundwaters in the overlying rocks. These hot groundwaters leach soluble elements from the surrounding rocks and redeposit them as hydrothermal minerals where conditions are favorable elsewhere in the hydrothermal system. Many of the world's precious and base-metal ore deposits are mined from ancient calderas, while geothermal energy is tapped from the superheated groundwaters circulating in younger ones.

As part of a program to answer basic scientific questions on explosive volcanism, hydrothermal dynamics, and mineralization, a scientific well (the deepest, hottest, continuously cored hole in North America) was drilled to 1762 m and 295°C in the youthful Valles caldera of northern New Mexico. Investigations are just beginning, but already the core and fluid samples from the hole are revealing scientifically exciting and tantalizing results. The core provides the first complete record of volcanic activity associated with the caldera, allowing researchers to unravel the complex sequence and nature of caldera eruptions. This information will be valuable in understanding the behavior of similar volcanic complexes around the world, and will enhance our capabilities to assess volcanic hazards. Additionally, the core bears a wide variety of hydrothermal minerals, some of which are currently being deposited by active hot groundwaters. These include zinc, iron, copper, antimony, and silver ore minerals. The opportunity to evaluate the physical chemistry of ore minerals and the fluids that deposit them has never been available before in the caldera environment, and these data will improve our understanding of how ore depositing systems work and our ability to locate and exploit such resources. Information from the core and the bore hole itself shows that the active hydrothermal system consists of a shallow steam-rich vapor cap overlying a superheated liquid water reservoir within caldera volcanic rocks. Evidence indicates that this shallow high temperature reservoir has evolved from a precursor hydrothermal system over the last 600,000 years. This

reservoir in turn overlies, but is largely separated from, another system of concentrated superheated liquid water which may contain components of waters actually derived from the crystallizing magma body some kilometers below. Thus, researchers studying the hydrothermal systems in this project will, in effect, monitor the development of high temperature geothermal systems over a significant period of time, evaluating the role of heat and mass transfer from the magma to the shallow crust and the influences of volcano development on the distribution of the energy resources. These findings should be applicable to similar environments globally, and will afford a more efficient strategy for exploration and development of high temperature geothermal systems.

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38. Infrared Spectroscopy and Stable Isotope Geochemistry of Hydrous Silicate Glasses

California Institute of Technology: E. Stolper and S. Epstein (EG/G)

A unique combination of infrared spectroscopy, stable isotope geochemistry, and high pressure-temperature experimentation has been applied to the study of water and carbon dioxide dissolved in silicate magmas (molten rocks) and glasses. This work has led to quantitative constraints on the thermal and chemical evolution of magmatic systems of the sort being evaluated as potential geothermal and magma energy sources. Measurements of the solubility of carbon dioxide in magma and of the partitioning of deuterium and hydrogen between molten rocks and volcanic gases were used to decipher the nature of degassing phenomena associated with two recent explosive volcanic eruptions in the western United States.

For the eruption of the Mono Craters in central California about 650 years ago, the amount of deuterium in the volcanic rocks indicates that the change in eruptive style from explosive to quiescent coincided with a change in degassing mechanism. Further, our study led to the unanticipated conclusion that magmas in this system were rich in carbon dioxide as well as water.

The second volcano illuminated by these results is the explosive eruption which occurred in Long Valley, California, about 900,000 years ago. Analysis of volcanic glass trapped in crystals indicates that gas bubbles in magmas erupted from shallow depth are richer in water while those from greater depth are richer in carbon dioxide. These results show that models developed for explosive caldera (collapsed craters) formation must take into account the contribution of dissolved carbon dioxide to the eruptive process.

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APPLIED MATHEMATICAL SCIENCES

39. A New Technique for Calculating the Properties of Atoms and Molecules
Lawrence Berkeley Laboratory: W. Lester

It has long been asserted that with a computer big enough and fast enough any property of any atom or molecule can be calculated with any desired degree of accuracy by numerically solving the Schroedinger equation. The critical

phrase in this assertion is "big enough and fast enough." To date, no computer has been built that is big enough and fast enough to treat any but the simplest of atoms and molecules with an accuracy approaching that achievable by direct measurements. Present day research in quantum chemistry is aimed at finding sensible approximations of known accuracy appropriate to specific atomic and molecular properties. One of the most helpful approximations is the separation of the effects of the outer, valence electrons which are responsible for most of the chemical properties of atoms and molecules, from those of the inner, core electrons. Heretofore, the effects of the core electron have been approximated with a so-called pseudopotential. Now, scientists at the Lawrence Berkeley Laboratory have found a new approach, based on a Monte Carlo approximation, for including the core electrons without a corresponding, prohibitively expensive increase in computational time. Monte Carlo methods are statistical methods for calculating properties at random, sample "points" and deducing the properties of the system through a statistical analysis of the sample. The approach of the Berkeley group treats the core electrons and valence electrons separately by establishing different time and energy scales for sampling the two sets of electrons. This approach, known as a damped-core quantum Monte Carlo method, has been applied to the calculation of the ionization potentials and electron affinities of carbon, silicon, and germanium with encouraging results. These properties agree with experimental values to within 2% while at the same time their calculation achieves a factor of 5000 decrease in computer time when compared to a full, traditional quantum Monte Carlo calculation. Using these advances and the Department's supercomputers at Lawrence Livermore National Laboratory will put many important chemical systems within reach of theoretical calculation.

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40. Time Stepping Algorithm for Parallel Computers Provides Multiplicative Speedups

Sandia National Laboratories/Albuquerque: D. E. Womble

Parabolic and hyperbolic differential equations are often solved numerically by time stepping algorithms, which are usually regarded as inherently sequential in time (i.e., the solution on a time level must be known before the computation of the solution at subsequent time levels can start). This research has demonstrated that it is possible for processors to perform useful work on many time levels simultaneously. Specifically, it is possible for processors assigned to "later" time levels to compute a very good initial guess for the solution based on partial solutions from previous time levels, thus reducing the time required for solution. The reduction of computer time used to get the final solution can be measured as parallel speedup. The parallelization of the time stepping algorithm is independent of any parallelism of the spatial algorithm and therefore the two speedup factors result in a multiplicative speedup factor.

This research project developed the theoretical and numerical implementation of an algorithm that combines both parallel iterations in time as well as space, allowing computation on many time levels simultaneously. Although the

time iterations are initially further from convergence, the effective number of iterations to convergence is much smaller, providing speedup factors that multiply any parallelism achieved in space variables.

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41. New Form of Carbon Dioxide Discovered Using Supercomputers
Ames Laboratory: K. Ruedenberg

During the past year, a new stable form of carbon dioxide has been discovered using a Cray supercomputer at the National Magnetic Fusion Energy Computer Center at Lawrence Livermore National Laboratory. The discovery was made by using an ab initio, quantum chemical calculation. In an ab initio calculation, properties such as structures and internal energies are calculated for atoms and molecules using only the knowledge of the charges and masses of the constituent nuclei and atoms. Because of the many particles involved (for carbon dioxide, 44 electrons and 3 nuclei) only calculations based on many simplifying assumptions have been performed in the past rendering the calculations useful for only the crudest of qualitative predictions. With the availability of very powerful and fast computers, it is now possible to perform quantum chemical calculations for small molecules with very few simplifying assumptions and with results that can be used for quantitative predictions with known accuracy. The calculation for carbon dioxide showed that a second form of the molecule exists, namely a triangle in which each atom is bonded to the other two. In the familiar form of carbon dioxide, the two oxygen atoms are each bonded only to the carbon atom. Although the new form is chemically unstable relative to the familiar form, the existence of another stable form has practical implications in combustion chemistry where the density of available energy states plays a critical role in determining the rates of chemical reactions. Of particular interest in this study is the fact that a large body of experimental data on the excited energy states of carbon dioxide existed, but a second form was not suspected. Even with the large amount of computer time (nearly 600 hours) required for this calculation, all possible configurations of the three atoms in carbon dioxide could not be considered. Even so, the calculation which showed the existence of the new form also hinted that yet a third form, C₀₀, might also exist.

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42. Prediction of New Low Compressibility Solids
Lawrence Berkeley Laboratory: M. L. Cohen and A. Y. Liu

New materials which are harder than diamond have been predicted by theoretical calculations. An empirical model and ab initio calculation of the bulk compressibility of covalent solids are used to suggest possible new hard materials. The empirical model indicates that hypothetical covalent solids formed between carbon and nitrogen are good candidates for extremely hard materials. A prototype carbon-nitrogen system was chosen, a form of based on the complex beta-Si₃N₄ structure, and a calculation of the total energy was made on the Department's Cray super-computers at the National Magnetic Fusion

Energy Computer Center. The calculations were consistent with the model and show the new material to have a bulk compressibility equal to or less than that of diamond. It may be possible to synthesize these novel materials in the laboratory.

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43. A New Monte Carlo Event Generator
Brookhaven National Laboratory: M. Creutz

A new Monte-Carlo event generator computer program named VENUS has been developed to simulate individual events for high energy nucleon-nucleon, nucleon-nucleus and nucleus-nucleus collisions. Ultra-relativistic heavy-ion collisions are such complicated events that there is little hope of finding quark-gluon plasma without detailed understanding of the reaction mechanism. In general perturbative methods cannot be used to calculate cross sections in this regime: one must rely on models that allow calculation of measurable quantities, models that can be seriously tested. VENUS uses the mechanism of color exchange between quarks and antiquarks of colliding nucleons to form colored strings. The total nucleus-nucleus collision becomes multiple color exchange leading to the formation of many strings. The decay of particles is then computed using other information developed at Brookhaven. String models of this type are the only ones able to explain most of the experimental data at this time. VENUS has been used to analyze data from the European Accelerator Laboratory (CERN) heavy-ion experiments. Studies are underway to investigate energies above those of the CERN experiments in contemplation of the proposed Relativistic Heavy Ion Collider (RHIC) on the Department's Supercomputers.

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ENERGY BIOSCIENCES

44. Light Regulation of Photosynthesis
University of California at Berkeley: W. Gruissem

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

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45. Development of Gene Transfer Technology for Sulfate Reducing Bacteria
University of Missouri: J. Wall

Sulfate reducing bacteria convert sulfate into H_2S during respiration instead of converting oxygen to H_2O as normally occurs in macroscopic organisms. These organisms play critical roles in the global sulfur cycle; metal corrosion; and in oil well souring, sewage treatment and other fermentation processes that take place in oxygen depleted environments. While there has been considerable progress in learning about specific steps in sulfate respiration in the sulfate reducing bacteria, the integration of these steps and the integration with the rest of the biological processes occurring within the bacteria have not been studied. One major approach to studying both the physiology and biochemical reactions of these bacteria would be the development of genetic and molecular biological tools.

A virus has been discovered that has the ability to transfer genes between various strains of sulfate reducing bacteria. Bits of DNA from the host cell are mixed in with the viral DNA when the virus is formed. When the virus infects another bacterial cell, the DNA is released in the new host cell and is incorporated into the genetic material of the new cell. The discovery of this system constitutes a major development in genetically characterizing these organisms. While a system that would permit the genetic transformation of these organisms (the introduction of totally foreign DNA into the bacterial chromosome) is still being sought, the development of the viral transfer system opens the door for extensive genetic studies on these important organisms.

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46. Novel Gene Found in Methane Producing Bacteria
Ohio State University: J. Reeve

The analysis of the structure or sequence of a particular gene or chromosome region sometimes gives insights beyond those which were originally planned. Such an example was the discovery, in the course of studies of the gene sequences encoding enzymes involved in the formation of methane in methane producing bacteria, of a gene sequence for which no function was known. By comparison of this gene to other gene sequences cataloged in the GenBank data base, it was discovered that the gene has the information for the synthesis of a polypeptide that could best be described as polyferridoxin. The polypeptide

should have the capacity to readily accept and give up six electron pairs. The physiological role of this molecule is not known, but there are several intriguing possibilities. These include behaving as a biological capacitor, being the equivalent of a biological electric wire, or serving as a ferridoxin precursor molecule. Studies are now under way to determine the biological role of the 'polyferridoxin' molecule in methane producing microbes.

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47. Visible Markers for Genetically Transformed Plants

University of Georgia: S. Wessler, and R. Ludwig; and Pioneer Hi-Bred Seed Company, Iowa

The technology available to insert foreign genes into one-celled organisms or cells permits success rates of incorporation varying from only one in one thousand to one in ten million. The minuscule size of individual cells means, however, that millions may be treated at one time. The major limitation becomes one of identifying cells which have received the foreign gene(s) or DNA fragment. A small gene with a rather pronounced effect, called a marker gene, if it can be incorporated along with the DNA fragment or gene of interest, is an essential tool for genetic engineering applications.

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

