SOME EXAMPLES OF ACCOMPLISHMENTS

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Table of Contents

14. Neutron Scattering Studies of the Collagen Spacing in Mineralized Bone
(Materials Sciences - Research at Oak Ridge National Laboratory's High Flux Isotope Reactor by S. Lees, Forsyth Dental Center, Boston, MA; L. C. Bonar, Harvard Medical School, Boston, MA; and H. A. Mook, ORNL)

15. Decoupling of Filaments in Superconducting Wire
(Materials Science-Ames Laboratory, D. K. Finnemore)

16. Mechanistic Characterization of an Electrocatalyst Prepared by Ion Implantation
(Materials Sciences-Oak Ridge National Laboratory, E. J. Kelly, C. E. Vallet, and C. M. White)

17. New Understanding of Electrical Contact Behavior in Advanced Semiconductors
(Materials Sciences-Lawrence Berkeley Laboratory, J. Washburn and R. Gronsky)

18. Improved Heat Transfer Performance Exhibited with Non-Newtonian Fluids
(Engineering and Geosciences - University of Illinois at Chicago, J. Hartnett)

19. Coolant "Dryout" Can Produce Severe Temperature Excursions
(Engineering and Geosciences - Northwestern University, G. Bankoff)

20. Electronic Structure and Bonding in Tantalum Carbide
(Materials Sciences-Oak Ridge National laboratory, G. R. Gruzalski and D. M. Zehner)

21. Low Emittance Lattice on the Positron Electron Project Storage Ring (PEP)
(Chemical Sciences and Materials Sciences - Stanford University, A. Hofmann, and coworkers)

22. Microcrystal Diffraction Structure Determination Using Synchrotron Radiation
(Materials Sciences and Chemical Sciences - Exxon, J. Newsam at BNL)

23. New Basis for Understanding the High Temperature Oxidation Resistance of Alloys
(Materials Sciences - Massachusetts Institute of Technology, G. J. Yurek)

24. Polarized Neutron Reflection: A New Technique for Study of Surface Magnetization
(Materials Sciences-Argonne National Laboratory, G. Felcher)

25. Implementation and Successful Utilization of the PEP Undulator Beam Line
(Chemical Sciences and Materials Sciences - Stanford University, research conducted by scientists from AT&T Bell Labs, Exxon, BNL, Hewlett-Packard, and Stanford University)

26. Chemical Anchoring of Dispersed Platinum in Zeolite Catalysts Discovered
(Chemical Sciences - Northwestern University, W. M. H. Sachtler)

27. Metal Clusters: Reactivity and Catalysis
(Chemical Sciences - Argonne National Laboratory, S. J. Riley et. al.)

28. Potential Application of Sound Wave Mixing to Determine Rock Structure
(Engineering & Geosciences - Los Alamos National Laboratory, R. Shankland)

29. Novel Optical Helium Afterglow Detector
(Chemical Sciences - Ames Laboratory, A. D'Silva)

30. Soft X-ray Laser Delivers Sizeable Amounts of Energy
(Advanced Energy Projects - Princeton Plasma Physics Laboratory, S. Suckewer)

31. Precision Lattice Parameters of Ni_3Al Alloys Reveal Crystallographic Defects
(Materials Sciences - Oak Ridge National Laboratory, C. J. Sparks, B. Calvin, G. E. Ice, and D. Kroeger; and Nagasaki University, Nagasaki, Japan, M. Hasaka)

32. Parallel Algorithms for Linear Algebra Applications
(Applied Mathematical Sciences - Argonne National Laboratory, J. Dongarra and D. Sorensen, and University of Illinois, A. Sameh)

33. Vectorization of GEANT Code
(Applied Mathematical Sciences - Florida State University, J. Lannutti)

1. RAPRENOx: A Process to Remove Nitrogen Oxides from Exhaust Gases

Scientists at the Combustion Research Facility (CRF) have recently developed a process, called RAPRENOx, for the removal of NOx from exhaust gases. The process was discovered while carrying out fundamental studies of the combustion chemistry of nitrogen. The feasibility of the process was demonstrated by using it to remove NOx from the exhaust of an experimental diesel engine. This process uses an inexpensive substance added to the exhaust stream from a combustor. The substance is cyanuric acid, commonly used for water treatment in swimming pools.

It is believed that RAPRENOx will be broadly applicable to combustion exhausts. A patent application has been filed for the process, and a waiver of patent rights has been granted to Dr. Perry, the inventor, in the interest of fostering rapid commercialization in the private sector.

(Chemical Sciences - Combustion Research Facility, Sandia National Laboratory/Livermore; R. A. Perry and D. L. Sieberg)

2. Transfer of New Magnetic Refrigeration Technology to Industry

A concept known as "magnetic refrigeration" was recently developed which offers the potential for reducing energy consumption in refrigeration processes. Magnetic refrigeration uses the so-called magnetocaloric effect: certain materials, when "magnetized" and "demagnetized" in a non-constant magnetic field, will cyclically absorb and release heat. The magnetization/demagnetization process is almost completely "reversible", which implies almost no energy loss in the cycle. When properly configured, such a system can be used to remove heat from, or cool, any "thermal load". At Los Alamos National Laboratory (LANL) a device with a capacity of about 1 watt, operating between 4.2 and 15^{o} K (degrees above absolute zero) was designed, fabricated and successfully tested.

Refrigeration usually requires a lot of energy, especially to attain extremely low temperatures. Compared to conventional gas-cycle refrigerators, magnetic refrigerators are projected to be more efficient, smaller, and more flexible in meeting specific design temperatures. Low temperature processes and applications that could benefit from a more efficient refrigeration process include gas liquefaction, superconducting magnets, and highly sensitive detectors of electromagnetic radiation.

In FY 1986, a transfer of the technology from LANL to private industry was effected. The Astronautics Corporation of America (ACA) offered to provide the necessary equipment, facilities, management, and financial resources for at least three years to develop commercial magnetic refrigerator products. The Principal Investigator on the magnetic cryocooler project along with three key staff members left LANL to work with ACA undertaking commercial development of magnetic refrigerators.

Since this transfer, the ACA staff working exclusively on magnetic refrigeration has been expanded to 15 people; more are being hired. An advanced, fully engineered prototype of a commercial magnetic refrigerator with a cooling capacity of about 1 watt, operating between 4.2 and 15° K is being fabricated.
(Advanced Energy Projects - Los Alamos National Laboratory, J. Barclay)

3. Key Enzyme for Ethylene Synthesis in Plants Isolated

Ethylene gas has been found to be an important regulator of plant growth. This past year, an enzyme (1-aminocyclopropane-1-carboxylate synthase) playing a key role in its synthesis was isolated and purified. The enzyme, which is present as only 1 ppm of the total protein in a plant, was successfully purified by chromatography and later isolated using "monoclonal antibody" techniques.

Ethylene is involved with both normal development of plants and responses to physical and biological stresses; thus the control of its synthesis is a crucial question in understanding plant growth. The isolation of this enzyme now opens the way to applying molecular biological methods to probe the question of how physiological factors activate or deactivate the gene that controls the reaction pathway for ethylene synthesis in plants.

(Biological Energy Research - Michigan State University, H. Kende)

4. Sinter-Forging of Ceramic Composites

Sinter-forging, a new process based upon a property called "superplastic deformation" and carried out at relatively low temperatures, has been used to press a mixture of alumina and titania powders to maximum compaction in a desired shape. The sinter-forging product is less subject to flaws and imperfections than one made using the conventional sintering process. Thus sinter-forging offers the possibility of enhnacing the reliability of ceramic components.

In this work, theory predicted and experiments demonstrated that sinter-forging, with its capability to simultaneously form and densify, is ideally suited for the fabrication of composites, a result that cannot be obtained through the conventional sintering process. Ceramic parts can be forged and densified with a minimum of imperfections or microcracks in a one step process.

Ceramics are traditionally fabricated by sintering, followed by machining. The conventional process consists of firing a ceramic powder at high temperature. During sintering the part densifies to near full density, resulting in dimensional shrinkage of typically 20 percent. The exact dimensions of the sintered part are limited by the precision with which the shrinkage can be predicted. This prediction is often difficult. Therefore, expensive machining, which also is a source of flaws to the final product, is necessary to obtain the exact dimensions. Machining can now be avoided by the one step sinter-forging process.

(Materials Sciences - Cornell University, R. Raj)

5. Chemist Provides Theory for Antarctic Ozone Hole

Annually, there is a temporary thinning of the earth's protective ozone layer over Antarctica; this phenomenon was first noted 10 years ago and is steadily worsening. Ozone concentration at the time of "thinning" is now 40% below the 1974 level. The phenomenon is puzzling and of concern to atmospheric scientists. Modeling studies carried out at the National Center for Atmospheric Research appear to support the hypothesis of F. Sherwood Rowland of the University of California, Irvine, that chlorofluorocarbons are depleting the earth's ozone layer. If correct, this hypothesis means that the large ozone depletions should be confined to the Antarctic in the spring and should continue to increase with release of chlorofluorocarbons to the environment.

The "hole" appears annually at the beginning of spring in Antarctica, in September, and recovers in November. A mechanism to explain the ozone observations has been proposed which involves a catalytic reaction between chlorine nitrate ($ClONO_2$) and hydrogen chloride gas or possibly water vapor. The mechanism takes into account (1) a high aerosol surface area to catalyze the reaction which occurs in polar stratospheric clouds predominantly between July and September, (2) the first rays of sunlight in early spring to photolyze the molecular chlorine reaction product to atomic chlorine, which subsequently attacks the ozone, and (3) the increasing total chlorine content of the atmosphere. In the Arctic winter, which is warmer, the polar stratospheric clouds are not as prevalent.

(Chemical Sciences - University of California, Irvine; F. S. Rowland)

6. Hydrogen Production From Water Using Green Plants

A novel composite material that links together photosynthetic and catalytic reactions was prepared this past year at Oak Ridge National Laboratory. Photosynthesis in green plants is carried out in chloroplasts which are made up of organic molecules that use light from the sun to produce carbohydrates from carbon dioxide and water. The particular molecule in the chloroplast that traps light is chlorophyll, while other complex molecules participate in the sequence of reactions that produce carbohydrates.

The reactions that occur during photosynthesis depend on electron transport at the molecular level. By coating the chloroplast with platinum, electrical contact can be made with the photosynthetic electron transport chain. This contact draws electrons away from the normal electron transport chain to the platinum which then catalyzes the formation of hydrogen and oxygen from the available chemical reactants.

The new composite material, the "platinized chloroplast", provides a novel solar energy driven system that produces hydrogen and oxygen. This solar-chemical approach is an example of using green plant biotechnology for fuel production from renewable resources.

(Chemical Sciences - Oak Ridge National Laboratory, E. Greenbaum)

7. Small Molecules Play Key Roles in Activating Genetic Messages

The genetic activity involved in the formation of nitrogen fixing root nodules of plants may be induced by the action of a naturally occurring compound known as luteolin, which occurs in the host plant root. This finding was reported in Science magazine in 1986.

This discovery fits into a pattern of recent findings, suggesting that a number of unique, relatively simple molecules (including carbohydrates) are critical in turning on important genetically controlled processes. The roles of simpler molecules in these functions have not been appreciated previously.

(Biological Energy Research - Stanford University, S. A. Long)

8. Enzyme to Breakdown Lignin Isolated and Genetically Engineered

In recent years, investigations have begun to define the biologically mediated breakdown of lignin. An enzyme with "ligninase" activity has been isolated from a wood rotting fungus. Using current molecular biological techniques, it has been possible to genetically transfer the "ligninase" gene from the fungus to a bacterium where it has produced new copies of the enzyme that had been isolated from the fungus.

This accomplishment now permits a detailed structural analysis of the gene and the enzyme product. It also opens the way for various modifications to enhance the level of ligninase activity, a prelude to potential developments on a commercial scale to utilize this renewable resource, second in abundance only to cellulose.

(Biological Energy Research - Michigan State University, A. Reddy)

9. Ion-Beam Smoothing of Mirror Surfaces

A process of "ion beam smoothing" to reduce the roughness of surfaces used for mirrors was demonstrated this past year at the Oak Ridge National Laboratory (ORNL). These mirrors have potential applications in areas such as space-based laser defense systems and in surveillance systems. For mirror applications, the smoothness of a surface is important in determining the quality and quantity of light that is reflected from a surface. At present, the smoothest mirror surfaces are fabricated by diamond machining followed by polishing; machining, however, is an expensive and time consuming process. In addition, some materials (like beryllium) are extremely brittle, oxidize easily, and are toxic. For such materials, fabrication of mirrors by conventional techniques is very difficult. Thus advanced, low cost techniques for producing smooth surfaces for mirror applications are needed. This process, called "Ion Beam Smoothing", has demonstrated great promise as a method to produce smooth surfaces. Research to develop this technique was carried out at ORNL in collaboration with scientists at Universal Energy Systems and the University of Nebraska.

Ion beam smoothing consists of using an energetic ion beam to bombard a surface. If moderate doses are used, the incident ions transfer energy to atoms on the surface, providing them with enough surface mobility so that the roughness of the surface can be reduced through atomic motion.

To date, surfaces of molybdenum, copper, and berrylium have been made smoother by the ion beam technique. In some cases, a reduction in the amount of scattered light by factors of up to 25 have been achieved. In addition to smoothing on an atomic scale, ion bombardment can also be used to passivate surfaces by ion implantation, to increase film adherence by ion mixing, and to alter subsurface microstructures by displacement damage. These techniques should be applicable to almost any surface.

(Materials Sciences - University of Nebraska, J. A. Woollan; Naval Weapons Center, China Lake, CA, J. Bennett; Universal Energy Systems, D. Ingram and P. Pronko; Oak Ridge National Laboratory, D. B. Poker, J. M. Williams, and B. R. Appleton)

10. Stanford Angiography Project

Images of the coronary arterial system of three human patients have been obtained using synchrotron x-rays at SSRL. In comparison with present techniques, synchrotron radiation imaging would be safe and economical and could drastically reduce the incidence of debiliating heart disease.

At the present time there are no alternative techniques for imaging human cardiovascular systems that do not pose a significant risk to the patient. Conventional x-ray angiography, requiring the catherization of the coronary arteries, is sufficiently dangerous and expensive that it is only used on patients with overt symptoms of heart disease, such as patients with angina or a history of heart attacks. Thus synchrotron radiation angiography appears to offer an alternative approach allowing patients to be routinely screened for heart disease before the onset of overt symptoms, and receive treatment sooner.

This result, made possible through BES' major user facility support, was accomplished by extracting a 120 mm wide polychromatic x-ray beam from the storage ring, subdividing it into two narrow monochromatic beams using silicon crystals, and measuring the relative absorption of the two beams with a position sensitive detector. The patients were administered, by injection, an iodine-bearing contrast agent which is highly opaque for one of the monochromatic x-ray beams . A digital subtraction of the two absorption profiles provides an image of the cardiovascular system, free from artifices due to, for example bone and dense tissue.

(Chemical Sciences and Materials Sciences support facility operations - Research conducted at the Stanford Synchrotron Radiation Laboratory by scientists from Stanford University, LBL, BNL and SSRL)

11. New Advanced Semiconductors

Vapor phase growth methods -- the deposition of controlled ratios of elements from the vapor phase onto a surface -- have been developed to synthesize wide ranges of novel alloys as new electronic materials. Gallium-arsenic-germanium alloys with a continuously variable range of composition have been grown on gallium-arsenide surfaces using ion bombardment during the vapor phase growth process. The growth of single crystal alloys of gallium-antimony-germanium, gallium-antimony-tin, and germanium-tin, representing three subclasses of metastable crystalline materials has been successfully demonstrated. Some of these alloys, such as gallium-antimony-germanium, have been investigated by a wide variety of techniques and have been found to exhibit unusual and appealing structural, optical, electronic, vibrational, and thermodynamic properties.

This work adds an important general new category of single crystal semiconductors that previously could not be prepared. These materials have led to new theoretical work that seeks to predict other single crystal semiconductors and to explain their unusual properties and behavior. This work has also increased interest in the use of low-energy accelerated dopant beams during the molecular beam epitaxial deposition of semiconductor devices to achieve better precision and reliability in control of dopant incorporation and concentration depth distributions. The latter is of critical importance to the semiconductor industry and the market that it responds to.

(Materials Sciences - University of Illinois, J. E. Greene)

12. Electron Capture Properties Used to Detect Explosives

A new, highly sensitive detector for explosives has resulted from research originally directed toward highly precise measurement of the properties of very low-energy electrons. The need for these measurements arose in studies of the rates and directions of air motion for energy conservation building design purposes. For commercial use, the detector has applications at airports and harbors, and at other locations where there is concern for the unauthorized presence of explosives. The Department of Transportation and DOE are now considering a proposal for further development of this new safety and security related technology.

The detection method exploits the large capture cross-sections that some complex molecules have for capturing very low-energy electrons. Recently it has been realized that among such complex molecules are those of certain common explosives. Negative ions formed by electrons that attach to the molecules are readily detected and identified. Thus, the research has yielded a useful, unanticipated bonus in the form of a new sensitive method of detecting explosives.

(Engineering and Geosciences - Jet Propulsion Laboratory, A. Chutjian).

13. Improved Models for Microcrack Formation

Research at Lawrence Livermore National Laboratory and the University of Wisconsin has led to improved computer models for predicting microcrack formation and resulting changes in mechanical properties of rock. The results from these studies will be of considerable use in the development of nuclear waste repositories or geothermal reservoirs. These energy technologies must deal with thermal effects from both natural and artificial processes.

The mechanical and hydrologic response of rock masses to heat is important in understanding fundamental geologic processes, such as the effect of a magmatic intrusion on the hydrothermal system of the surrounding country rock. Thermal stresses cause microscopic cracks in rock that can weaken its mechanical strength and alter its permeability.

In the newly developed models, thermally produced cracks are attributed to different rates at which rocks expand when heated. Each mineral is treated as a sphere in a matrix whose intrinsic properties are an average of the properties of all the minerals. This model predicts mechanical behavior for different and changing combinations of pressure and temperature conditions. Application of pressure before adding heat tends to suppress thermal cracking. The model has been validated for a variety of rock types, including several granites where large scale heater experiments have been conducted.

(Engineering and Geosciences - Lawrence Livermore National Laboratory, University of Wisconsin, H. Wang)

14. Neutron Scattering Studies of the Collagen Spacing in Mineralized Bone

Collagen, a long, chain-like molecule, is the principal organic component of bone, constituting about 30% of its weight. The collagen forms a regular array whose spacing can be measured by x-ray diffraction in demineralized bone. The strength of the bone is provided by minerals that crosslink collagen molecules so they cannot slide past each other. The collagen spacing cannot be studied by x-rays in mineralized bone because x-rays are strongly absorbed and scattered by minerals in the bone. However, collagen spacing is easily observed in mineralized bone by neutron diffraction, because neutrons are not strongly affected by the minerals. Study of collagen in bone is essential to understand mineral deposition in bone formation and mechanisms that cause mineral loss or osteoporosis. Results demonstrate how mineral cross-linking takes place in bone formation and how it can be inhibited by a particular drug, β - aminopropionitrile. Studies of the effect of vitamin C on bone formation are in progress, as are studies on the mechanism of osteoporosis.

(Materials Sciences and Chemical Sciences - Research at Oak Ridge National Laboratory's High Flux Isotope Reactor by S. Lees, Forsyth Dental Center, Boston, MA; L. C. Bonar, Harvard Medical School, Boston, MA; and H. A. Mook, ORNL, Oak Ridge, TN)

15. Decoupling of Filaments in Superconducting Wire

In superconducting magnet conductor materials, it is important to have fine filaments of niobium-titanium alloy embedded in copper to provide well defined magnetic field shapes or profiles. Typical filament diameters are 2.5 micrometers (1/10,000 inch), and the copper barrier separating the filaments might be 0.3 micrometers in, for example, magnets for the Superconducting Supercollider. At these extremely small dimensions, there can be a substantial coupling of the supercurrents flowing in the filaments and a negative impact on the magnetic field shape unless the materials are carefully engineered to quench or eliminate these currents.

This research provides a quantitative basis for solving this problem using an experimentally verified model. The model is for the supercurrent coupling between filaments as a function of temperature, magnetic field, and both magnetic impurity and non-magnetic impurity scattering rates. It shows quantitatively how to quench these undesirable effects with magnetic impurities, and procedures have been developed to accomplish this. Thus conductor designers can now specify the magnetic impurity content needed to eliminate the undesirable supercurrents at any given temperature, magnetic field and non-magnetic impurity content.

(Materials Science - Ames Laboratory, D. K. Finnemore)

16. Mechanistic Characterization of an Electrocatalyst Prepared by Ion Implantation

Ruthenium ions were implanted into the surface of titanium metal. Oxidation of the implanted surface gave a ruthenium-titanium oxide coating about 3 nm (1/10,000,000 inch) thick. This composite electrode showed a 10,000-fold enhancement in the rate of chlorine gas evolution from acidic chloride solutions when compared with unmodified titanium. Photoacoustic and photocurrent spectroscopy of the working electrode confirmed that the mixed oxide overlayer had the metallic conductivity required for efficient electrocatalysis.

A ruthenium-titanium mixed oxide coating on titanium metal is the electrode used for production of chlorine in the chloralkali industry. Such coatings are normally prepared by a succession of depositions of metal salts followed by open flame heating. This work shows that electrocatalysts of the same composition can be prepared by ion implantation techniques. The electrodes prepared by ion implantation and surface oxidation are also proving to be very well-behaved for studies of the catalytic mechanism itself. Ion implantation, with its excellent control of composition, permits comparative mechanistic studies to be made of titanium mixed-oxide electrodes which cannot be prepared otherwise. Such information is needed to understand and optimize the role of mixed oxide electrocatalysts.

(Materials Sciences - Oak Ridge National Laboratory, E. J. Kelly, C. E. Vallet, and C. M. White)

17. New Understanding of Electrical Contact Behavior in Advanced Semiconductors

Some reasons have been found to explain why forming certain kinds of microscopic electrical contacts to gallium-arsenic semiconductors has proven difficult. A systematic investigation has been made, using high resolution transmission electron microscopy and microanalytical techniques, of the solid state reactions that take place when a metal is deposited on the surface of a semiconductor single crystal wafer. The important findings include: (1) the first new phase to appear is often not the equilibrium phase but one that has a more favorable geometric fit to the available surface, (2) the uniformity of the final reacted film depends critically on events during the early stages of the reaction and how they affect diffusion and 3) a thin oxide layer on the semiconductor surface can behave as a diffusion barrier and lead to very non-uniform film growth.

The powerful capabilities of cross-section high resolution transmission electron microscopy (TEM) have been demonstrated in the identification of phases on the surfaces of the semiconductor wafers studied. TEM techniques show the orientation relationships and the spatial distribution of the phases, the structure, and the composition. This research is providing information of major importance to the use of the gallium-arsenic class of semiconductors in the electronics industry.

(Materials Sciences - Lawrence Berkeley Laboratory, J. Washburn and R. Gronsky)

18. Improved Heat Transfer Performance Exhibited With Non-Newtonian Fluids

Sir Isaac Newton suggested that fluid behavior can be described by viscosity, a property that expresses how much a fluid will resist being moved or deformed. If a fluid has the same viscosity no matter how fast it is being deformed, it is called "Newtonian." Any departure from this behavior is "non-Newtonian." Research at the University of Illinois on working fluids for heating and cooling systems has recently found that, for relatively slow flow through a rectangular duct, certain non-Newtonian fluids transfer heat more than twice as effectively as Newtonian fluids at the same conditions.

Examples of non-Newtonian behavior include plastics, when they are forced through tubes before being molded into various useful shapes, and streams of foodstuffs in a water mixture, such as catsup. Other examples include paints, crude oil, printers ink, and toothpaste.

Besides knowing how much energy must be used to pump non-Newtonian fluids, it is important to understand their heat transfer behavior compared to that of common Newtonian fluids, such as water and all gases. Understanding this phenomenon will help improve the design of future, efficient heat exchangers when other considerations restrict working fluid flow rates.

(Engineering & Geosciences - University of Illinois at Chicago, J. Hartnett)

19. Coolant "Dryout" Can Produce Severe Temperature Excursions

A major problem facing the utility industry in the next decade is the probability of extensive tube failures in pressurized water nuclear power plant steam generators (boilers). An example is the recent failure at the Ginnay power plant, New York, caused by corrosion and thermal cycling. Alternate drying and rewetting can occur in the narrow gaps where tubes pass through support plates. Local drying within these gaps can enhance corrosion and cause severe surface temperature increases.

The first and only studies of convective boiling in extremely narrow gaps is continuing at Northwestern University. This work has found that the mechanism of heat transfer changes at a film thickness of 0.008 inch. Above this film thickness the heat transfer surface is covered by a thin liquid film with high heat transfer rates and stable surface temperatures. Below it, drying and rewetting cause frequent and high surface temperature fluctuations that lead to high stresses and enhanced corrosion. In addition to identifying this critical film thickness phenomenon, Northwestern researchers have modified boiling-heat-transfer correlations used in engineering design, to account for the film thickness effect. The ability to evaluate potential drying/rewetting conditions in power plant steam generators and to lessen the probability of their occurrence by proper design is extremely important to power plant engineers. Costs to repair such systems can be as high as $200 million. Drying may also occur in electronic packages where liquid coolants flow in narrow gaps between closely spaced power-dissipating components. In these cases a rapid temperature rise may cause poor operation or failure of the device.

(Engineering and Geosciences - Northwestern University, G. Bankoff)

20. Electronic Structure and Bonding in Tantalum Carbide

The properties of tantalum carbide are not only of fundamental interest, but they also are useful technologically. For example, tantalum carbide is superconducting, extremely hard and strong, chemically inert, has the highest melting point known, and it exists as a face-centered cubic material over a wide range of stoichiometry. Because the properties of tantalum carbide are strongly dependent upon carbon content, it is imperative to know how composition influences electronic structure and bonding.

The electron energy levels of tantalum carbide have been observed to change with the concentration of carbon. As carbon was removed preferentially from a tantalum carbide surface, the binding energies of the tantalum electrons, and the number of higher energy electron states increased. These changes have been explained in terms of (1) an increased electron density in the vicinity of the tantalum atoms resulting from carbon vacancies, (2) a corresponding redistribution of the tantalum electronic states, and (3) a transfer of electrons away from the remaining carbon atoms.

This work has considerably advanced the understanding of the electronic structure and bonding in tantalum carbide, and has provided a critical insight into the fundamental origins of the material's unique physical properties. Until now, little has been accomplished to provide such information.

(Materials Sciences - Oak Ridge National laboratory, G. R. Gruzalski and D. M. Zehner)

21. Low Emittance Lattice on the Positron Electron Project Storage Ring (PEP)

A new, low emittance lattice for the PEP storage ring, which uses existing magnets and power supplies, has been successfully implemented for synchrotron radiation experiments. A beam current of 4 milliamperes was accumulated in only 16 hours of machine physics. A measurement of an upper bound to the emittance yielded a value of 10 ± 1.5 nanometer-radians at 8 GeV. Emittance is a measure of the energy loss in the storage ring; the lower the emittance, the brighter the light. This is the lowest emittance achieved thus far on a storage ring on which synchrotron radiation research is performed. It is comparable to emittances currently under discussion for future storage ring designs for producing synchrotron radiation.

This success indicates that PEP can provide ultrahigh brightness synchrotron radiation before the new specially designed facilities become available over the next several years. The achievement of 4 milliamperes in such a short time implies that considerably higher currents will be achieved. This lattice will provide the opportunity to test and develop wigglers and undulators, as well as x-ray optics, for the planned facilities. The lattice also provide new capabilities for advanced research such as: (1) inelastic x-ray scattering to probe electronic and vibrational excitations of solids, (2) structural studies of surfaces and surface layers, (3) x-ray microprobe chemical analyses of extremely small volumes, and (4) atomic arrangements in extremely small crystals.

(Chemical Sciences and Materials Sciences support facility operations - Stanford University, Research conducted by A. Hofmann and coworkers from SLAC and SSRL.)

22. Microcrystal Diffraction Structure Determination Using Synchrotron Radiation

Zeolites are in wide commercial use as ion-exchangers, as sorbents, and in hydrocarbon conversion catalysis and separations. For example, they are used in Fluid Catalytic Cracking of crude oil, and in converting methanol to gasoline. Each use relies on the particular character of the zeolite's cage structure, a detailed knowledge of which is needed to understand the zeolite's properties and performance. Synthetic zeolites, however, are invariably microcrystalline with particle sizes of 10 microns (1/2500 inch) or less being typical. As a result, zeolite structural information has been limited to that which can be extracted, with difficulty, from data from powder samples.

On the Exxon beam lines at Brookhaven National Laboratory's National Synchrotron Light Source, microcrystal diffraction, a technique exploiting the brightness of the NSLS bending magnet x-ray source for measuring diffraction data from individual particles smaller than 10 microns is being developed.

The intense brightness of the sychrotron source has enabled measurements from zeolitic microcrystals at least 10,000 times smaller in volume than are accessible conventionally. This establishes the feasibility of a new tool for catalysis research and design. This accomplishment is an important example of the benefits to be gained under our Major Facilities User Program.

(Materials Sciences and Chemical Sciences support NSLS facility operations - Exxon, J. Newsam)

23. New Basis for Understanding the High Temperature Oxidation Resistance of Alloys

For the first time, the migration of impurity ions to grain boundaries in protective oxide films formed during the oxidation of alloys at high temperatures has been measured. This work is expected to have a large impact on the directions of future research and thinking in the area of high temperature oxidation, and to provide novel insights into the mechanisms of how protective oxide films form at high temperatures.

Also, based on these results, one can envisage the selective doping of oxide grain boundaries by modification of the alloy composition or the environment to improve the intrinsic properties of the oxide film, or to counteract the effects of harmful, segregated impurities at grain boundaries that otherwise control the oxidation process.

In the experiments conducted, it was shown that migration of sulfur and yttrium to grain boundaries in chromia films reduces the rate of alloy degradation by reducing the rate of film growth by 10 to 100 times. Migration of sulfur to grain boundaries in alumina films, on the other hand, increases the rate of oxidation by a factor of four.

The segregation of yttrium to grain boundaries in chromia films can be used to explain for the first time many of the beneficial effects of rare earth elements on oxidation resistance, and it is expected that knowledge of this effect will eventually lead to considerable improvements in the lifetimes of commercial alloys.

(Materials Sciences - Massachusetts Institute of Technology, G. J. Yurek)

24. Polarized Neutron Reflection: A New Technique for Study of Surface Magnetization

Until now, studying surface magnetization has been almost impossible. Now a nondestructive method for direct microscopic probing of the magnetism in surface layers has been developed. It has been successfully used to map field penetration in superconductors and magnetic depth profiles in recording devices that use layered magnetic materials. The technique uses a pulsed neutron source and exploits the spin-dependence of the reflectivity for spin-polarized neutrons. Experiments on superconducting niobium and lead confirmed expectations for the technique and also found behavior in lead-bismuth alloys not predicted by long-accepted theory. A major difference was found between the magnetic profiles of Fe_3O_4 and α-Fe_2O_3 in that the latter has a "magnetically dead" layer. In a recording device prototype with 20Å ferromagnetic and anti-ferromagnetic layers, a region of reduced antiferromagnetic moments extending some 600 Å below the surface was detected.

Polarized neutron reflection is the first technique that can provide nondestructive microscopic magnetization information over the range 20-500 Å from a surface. In basic research, polarized neutron reflection is the only method to directly test theories of surface phenomena in superconductivity, and despite 50 years of effort in magnetization, unexpected behavior which has an impact on the theory of

superconductivity was seen in Pb-Bi alloys. In applied research it is likely to prove revolutionary in characterizing magnetic multilayers. IBM has shown interest, is providing samples, and intends to support a research associate. Three European laboratories plan major efforts using a copy or adaptation of the instrument.

(Materials Sciences - Argonne National Laboratory, G. Felcher)

25. Implementation and Successful Use of the PEP Undulator Beam Line

The first x-ray undulator beam line implemented on the PEP storage ring is an order of magnitude brighter than any other x-ray beam line in the world. Two initial experiments immediately demonstrated the unparalleled experimental capabilities of such extremely bright beams. The structures of amorphous films as thin as 100 angstroms (0.0000004 inches) were studied using grazing incidence scattering. For a second experiment, a powerful high resolution (40 meV) inelastic x-ray scattering technique was developed and used.

The high brightness of this PEP beam line allows important new classes of experiments that have heretofore been impossible. The grazing incidence scattering experiments on PEP, for example, showed that it is possible to study thin poorly crystallized surface layers. This work could lead to better understanding of such scientific and technologically important phenomena as oxidation, corrosion, and wear. Extreme brightness is required for three reasons: (1) the sample's cross-section in grazing incidence is very small, (2) the beam must be highly parallel to optimize surface sensitivity and (3) amorphous materials are very weak scatterers. High brightness is also required for inelastic scattering experiments. These unique beam characteristics promise more detailed knowledge than ever before of electronic and vibrational excitations in solids.

(Chemical Sciences and Materials Sciences support facility operations - This body of work was carried out by G. Brown, SSRL, P. Fluoss, AT&T Bell Labs, and D. Moncton, Exxon and their collaborators at Exxon, BNL, Hewlett-Packard, and Stanford University)

26. Chemical Anchoring of Dispersed Platinum in Zeolite Catalysts Discovered

A new method has been discovered to keep catalytic metal particles, which have been introduced into a zeolite, from agglomerating at the higher temperature encountered in catalytic processes. This discovery is expected to be useful in a broad range of chemical processes including petroleum refining and chemical production from synthesis gas.

The chemical anchoring of the small catalytic platinum particles with cations of iron or chromium inserted into the zeolite structure was found to maintain the highly dispersed state of the platinum and thus to retain its catalytic activity. It has proved difficult in the past to prevent a highly dispersed metal within a zeolite from agglomerating into large particles at temperatures necessary for use as a catalyst.

A patent application based on this discovery has been filed by Professor Sachtler.

(Chemical Sciences - Northwestern University, W. M. H. Sachtler)

27. Metal Clusters: Reactivity and Catalysis

Scientists at Argonne National Laboratory are using a unique laser-vaporization source to produce metal clusters ranging from two to several hundred of atoms. These studies will undoubtedly lead to deeper understandings of catalysis and the adsorbate-surface interaction. Striking observations include remarkable changes in chemical reactivity with cluster size.

Classical heterogeneous catalysis or surface chemistry studies of metals involve examination of systems consisting of huge numbers of atoms. It is now possible to investigate chemical and physical properties of typical nickel, iron or cobalt metal catalysts on an atomic and molecular level by use of metal "clusters". The cluster source at Argonne is coupled to a gas reactor that permits controlled study of the reactions of added gases with the various clusters. Reaction products are detected by mass spectroscopy. Initial studies have focused upon the reaction of iron clusters that pertain to catalytic hydrogenation, oxidation, and ammonia synthesis processes.

(Chemical Sciences - Argonne National Laboratory, S. J. Riley et. al.)

28. Potential Application of Sound Wave Mixing to Determine Rock Structure

Basic research in rock physics at Los Alamos National Laboratory has revealed how two narrow beams of high, but different, frequency sound waves interact in rock to produce a narrow beam at their much lower difference frequency. The difference frequency beam thus created has the narrow width of the generating beams but can travel much farther in the rock because of its lower attenuation.

A controlled, narrow, low frequency, difference acoustic beam might be used to explore the earth's subsurface with greater range and without the ambiguities of conventional seismology, which uses undirected sources, such as transducers or explosives, that broadcast energy in an almost spherical pattern. This knowledge can be used to construct devices to show that acoustic energy can be radiated outward from boreholes, mine interiors, or the surface in either thin planes or narrow searchlight-like beams. Technology based on this phenomenon could reveal structure, stratigraphy, and in situ fluid conditions far better in many geological settings than is now possible.

A critical step was achieved this year with full verification of the selection rules that govern the angular relationships between the high frequency generating beams and the low frequency difference beam. This is the first confirmation of such an effect in rocks.

(Engineering and Geosciences - Los Alamos National Laboratory, R. Shankland)

29. Novel Optical Helium Afterglow Detector

Measurement of very low concentrations of specific components of complex samples such as fossil fuels has become much easier with the discovery of the helium afterglow detector. This device uses the phenomenon that creates the Aurora Borealis; the formation of long-lived excited species in an electrical discharge followed by the emission of light. The detector can be attached to a chromatograph, which splits mixtures into their components, allowing a complete compositional analysis of fossil-derived samples, waste streams, and other complicated samples. It is possible to simultaneously measure amounts of less than a billionth of a gram of mercury, sulfur, chlorine, bromine, and iodine.

Compared to previous devices for making these measurements, the new device offers unattended operation, low consumption of expensive discharge gases such as helium, and wide linear response from trace amounts to very high concentrations. The detector was discovered and developed by chemists at Ames Laboratory, and has recently become available commercially through CETAC Technologies. (The two organizations received an IR-100 award for the device in September, 1986).

(Chemical Sciences - Ames Laboratory, A. D'Silva)

30. Soft X-ray Laser Delivers Sizeable Amounts of Energy

There are many important uses for unique, high-intensity, laser produced x-rays in medicine, physics, biology and technology. In this work, for the first time a soft x-ray laser delivered energies useful in microscopy and holography.

In 1984 Princeton University scientists announced the first demonstration of a laboratory-scale laser active in the soft x-ray region. The following year, multilayered mirrors were used to enhance the x-ray emissions from the laser. In 1986, a 182 Å laser delivered 1 millijoule per pulse in a very finely collimated beam.

At the heart of the Princeton x-ray laser is a fast-recombining plasma. Initially, the plasma temperature is increased until the carbon atoms become completely ionized. The plasma then cools rapidly by intensive radiation losses, causing ions to recombine with free electrons. Because recombination occurs primarily at the higher energy levels while lower levels do not capture electrons, an excess of high-energy electrons develops. When these high-energy electrons "avalanche" to lower levels, x-rays are given off in the process. The lasing process occurs when the x-ray photons produced in this fashion stimulate the emission of additional photons from other ions, initiating a chain reaction resulting in an intense, highly focused x-ray pulse of a single wavelength.

(Advanced Energy Projects - Princeton Plasma Physics Laboratory, S. Suckewer)

31. Precision Lattice Parameters of Ni_3Al Alloys Reveal Crystallographic Defects

By adding small amounts of boron to extremely brittle metal alloys, such as the intermetallic alloy Ni_3Al, these materials can be altered so they can be hammered into thin sheets or drawn out into thin wire. These altered materials could be useful for many applications including heat exchangers, combustion chambers, turbines, and engines. This is the first of a series of studies of these defects with synchrotron radiation and is part of a larger effort to understand the basic principles of how boron can turn a brittle alloy into a malleable and widely useful high-temperature material. This study also demonstrates the value of synchrotron radiation in research of this kind.

The goal is to understand why boron additions of as little as 5 boron atoms per 10,000 nickel and aluminum atoms can make a ductile material out of one so brittle that it falls apart on fabrication. Among several studies aimed at understanding the effects of boron is the use of synchrotron radiation at the National Synchrotron Light Source (NSLS) to determine both the precise lattice expansion caused by these small additions of boron and the kind of defects producing the tetragonal distortions in these alloys. The high intensity and extremely tight collimation of synchrotron radiation produces a 1000-fold improvement in our ability to detect these changes.

The lattice parameters for rapidly quenched alloys near the composition Ni_3Al were determined at the NSLS, with boron shown to have a large expanding effect on the lattice. In addition, the deviations of the lattice parameters from a straight line reflect either magnetostriction in the paramagnetic alloy or changes in the number and kind of defects present.

(Materials Sciences - Oak Ridge National Laboratory, C. J. Sparks, B. Calvin, G. E. Ice, and D. Kroeger and Nagasaki University, Nagasaki, Japan, M. Hasaka)

32. Parallel Algorithms for Linear Algebra Applications

In addition to restructuring existing algorithms (step-by-step methods for solving problems) and developing tools to make it easier to use high-performance computers, scientists are investigating new classes of algorithms especially designed for highly parallel computers, machines that use more than one processor at a time, to segment a problem and work on more than one segment at the same time.

Recently, Argonne researchers developed a new algorithm for the "symmetric eigenvalue problem", one of the most fundamental problems of computational mathematics. "Symmetric eigenvalue problems" constitute the heart of many computational science applications. The performance of the parallel algorithm is impressive. Compared with the standard algorithm, the new algorithm is much faster, with the speedup becoming more dramatic as the size of the problem increases. In problems of order 500, for example, speedups of 15 have been observed on the CRAY X-MP-4, and speedups of over 50 recorded on the Alliant FX/8 supercomputer.

Most startling, however, is the speedup in serial mode of execution -- the way non-parallel machines solve problems. The algorithm offers significant improvement over the best sequential algorithm on large problems, and is also effective on problems of moderate size (order greater than 30) when run in serial mode. These results are surprising because the synchronization and computational activity needed to split a problem into parallel parts usually slows down performance.

(Applied Mathematical Sciences - Argonne National Laboratory, J. Dongarra and D. Sorensen, and University of Illinois, A. Sameh)

33. Vectorization of GEANT Code

The GEANT program, written by the CERN Data Handling division, is used extensively in the experimental high energy physics community. GEANT simulates particle-detector response, generates events from known theoretical input, and fabricates "Monte Carlo" data, which is then passed through the entire data reduction and analysis streams. Accurate simulation requires tracking every particle through detection elements. At peak intensities, electromagnetic interactions can result in tens of thousands of particles to be tracked.

Researchers at the Supercomputer Computations Research Institute (SCRI) at the Florida State University (FSU) recently developed an algorithm (step-by-step method for soving a problem) that demonstrated the validity of vectorization techniques for this track finding problem for a fixed target Detector experiment at Fermilab. Based on this success, the CERN Data Handling division and the SCRI researchers entered into a collaborative effort to apply these vectorization techniques to the widely used GEANT code. Although this work has only recently been undertaken, factors in speed up for portions of the GEANT code of 7 over scalar, non-vector versions have already been realized.

Currently, both CERN and Fermilab are preparing for major experiments on new facilities, and this work will significantly reduce the time required to process and to analyze data from these experiments. Additionally, this work verifies the utility and cost effectiveness of supercomputers for a large computational requirement that had previously been considered inappropriate for supercomputers.

(Applied Mathematical Sciences - Florida State University, J. Lannutti)