SOME EXAMPLES OF ACCOMPLISHMENTS

UNDER THE BASIC ENERGY SCIENCES

PROGRAM DURING 1983

FEBRUARY 15, 1984

Some Examples of Accomplishments Under the Basic Energy Sciences

Program during 1983

(February 15, 1984)

The Basic Energy Sciences Program supports about 1200 research projects. The following selections, while not fully reflective of the full range of activities under the program, are examples of how basic research can contribute to solving a wide variety of energy problems.

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1. Control of Structure and Properties of Ceramic Surfaces by Ion Implantation Shown

It has been demonstrated that the structure and surface hardness of ceramic surfaces can be modified and controlled by means of ion implantation to yield surface hardnesses that are greater or less than that of the original ceramic.

Results for ion-implanted alumina showed a hardness increase of 15 to 50% and a scratch-wear resistance increase of 30% as a consequence of ion implantation with chromium, nickel, iron, titanium or zirconium ions. The principal mechanism of implantation hardening was found to be due to implantation-induced structural damage on the aluminum sublattice, with some contribution from implantation damage on the oxygen sublattice.

The hardness also can be made to decrease during post-implantation thermal annealing of aluminum oxide; the mechanism was found to be associated with the recovery of the implantation-induced damage on both the aluminum and the oxygen sublattices. The implantation of alpha-phase silicon carbide with chromium or nitrogen caused the implanted surface region to become amorphous at implantation fluences above a certain critical level. This transformation from the crystalline to an amorphous state is accompanied by a decrease in hardness of 15 to 25%, an increase in fracture toughness of 30 to 40%, and an incease in scratch wear resistance of up to 70%.

This work established the feasibility of using ion implantation to systematically alter the structure and properties of ceramic surfaces. It has also demonstrated that control of the resultant structure may be achieved by the variation of implanted ion species, implantation temperature, and post implantation heat treatment.

(Oak Ridge National Laboratory, C. J. McHargue, B. R. Appleton, C. W. White, and J. M. Williams)

2. Selective Catalytic Conversion of Methanol to Ethanol Discovered

A new catalyst system has been discovered for conversion of methanol to ethanol. The system has several practical advantages over existing methods. Starting with methanol produced from coal, dry ethanol, which has higher fuel value per unit volume than methanol, is produced. The catalyst is based on iron pentacarbonyl in the presence of a tertiary amine. The principal co-product formed is carbon dioxide, rather than water as in existing methods which use a cobalt/carbonyl catalyst. Eliminating water is particularly beneficial because it can save the costly drying step.

In addition to not producing water, the iron system catalyzed reaction only requires half as much expensive hydrogen as in the cobalt/carbonyl catalyzed system. The selectivity of the iron/amine catalyst is virtually 100% for converting methanol to ethanol. There are no higher alcohols, alkyl acetates or acetals formed, in contrast to the cobalt systems, and this simplifies product purification considerably.

A mechanism for the iron/amine catalyzed reaction has been established through detailed chemical and kinetic studies. This understanding has led to development of a mixed catalyst, $Mn_2(Co)_{10}/Fe(Co)_5$/amine, which has both activity and selectivity superior to either metal carbonyl alone.

(Argonne National Laboratory, J. W. Ratkhe & coworkers)

3. Glow Discharge Implanted, Laser Annealed Silicon Single Crystals Produce Simple, High Efficiency Solar Cells

Simple, low-cost, yet very high efficiency solar cells have been produced from single crystal silicon by glow discharge implantation doping followed by pulsed laser annealing. This method involves two well understood processing steps, is easily automated and could radically change the manufacture of solar cells.

The cells are fabricated from standard phosphorous-doped single-crystal silicon wafers. A p-n junction is formed by implantation of boron followed by pulsed high-power laser illumination to activate the implanted atoms and anneal any implantation damage. A back surface field is created to reflect minority carriers back to the p-n junction area by deposition of a thin layer of antimony followed by illumination by laser pulses to cause inward diffusion. The cells are completed by cutting the wafers into desired sizes, applying contacts and antireflection coatings. The process is simple, though subtle, and efficient. It uses laser annealing and an inexpensive glow discharge boron implantation technique, both of which are easily automated and capable of high production rates. There is no high temperature processing, which is usually difficult and poorly controlled.

This development has led to three patent applications, two of which already have been granted, and the development of a XeCl laser system by an American company for automated high-production rate laser processing of these solar cells. Efficiencies of about 16.5% for these cells were measured by the Solar Energy Research Institute and found to be higher than that of any solar cell ever tested under the same conditions.

(Oak Ridge National Laboratory, R. T. Young & coworkers)

4. New Thin Film Photoelectrode Uses Visible Light to Generate Electricity or Split Water

One micron films of intrinsic (undoped) amorphous hydrogenated silicon deposited on stainless steel have been investigated as photocathodes in photoelectrochemical cells. The hydrogenated silicon was synthesized at RCA and its behavior characterized at MIT. The photoelectrodes are rugged, efficient and inexpensive.

The efficiency of the photocathode for converting visible light to electricity is in the 1-2% range, which is only about one-third less than efficiencies attained using expensive single crystal electrodes under the same conditions. Even more promising is the observation that this type of electrode produced a photovoltage more than 50% greater than that produced using a single crystal electrode. The efficiency for generating hydrogen by photoassisted electrolysis of water is equal to that obtained with the best single crystal electrodes.

Many advances reported in photoelectrochemical energy conversion in the past two years have been obtained with use of ultraviolet light, a less intense part of the solar spectrum at the earth's surface. This set of advances, in contrast, used the much more abundant visible part of sunlight. Research continues to increase further both our scientific understanding of these phenomena and the efficiencies of functioning of the new type of electrodes.

(Massachusetts Institute of Technology, M. Wrighton)

5. First Mu Meson Catalyzed Fusion Reaction Rate Measurement

In conventional approaches to fusion, hydrogen gases are heated to extremely high temperatures to form a plasma so that fusion reactions occur, releasing energy. Thirty-five years ago, it was suggested (by F.C. Frank and independently by Andrei Sakharov) that an elementary particle known as the muon could serve to catalyze the hydrogen fusion reaction so that it could proceed without the need for high temperatures. This process is therefore called cold fusion or muon-catalyzed fusion.

The basis for muon-catalyzed fusion is as follows. The negatively-charged muon behaves like a heavy electron and can substitute for an electron in a hydrogen atom. The muon is 200 times as heavy as an electron, and because there is an inverse relation between the mass of the negative particle and the radius of the atom, the muonic atom molecule is 200 times smaller than an ordinary hydrogen atom. The reduced size of the muonic atom brings the hydrogen nuclei so close together that they interact and fuse very soon after the muonic molecule forms. Indeed, the conditions inside a muonic hydrogen molecule are similar to those found inside a white dwarf star!

In this research, muons are introduced into a mixture of hydrogen gases (deuterium and tritium). Gas temperatures range from -280° F to 530° F, so the gases are very cold compared to plasmas. The muons replace electrons to form muonic hydrogen molecules and fusion ensues immediately. The muon is then free to catalyze other fusion reactions. Up to seventy (70) fusions per muon (average) have been observed in initial experiments. This is greater than expected but still insufficient for net power production. It has also been observed that the rate of the reactions increases with temperature (up to 530° F so far). However, it is clear that no thermal runaway or explosion is possible with this process.

Muon-catalyzed fusion research is continuing with Department of Energy support and similar research is also beginning in Europe and the Soviet Union. The research will provide answers to recurring questions regarding the possibility of practical applications for muon-catalyzed fusion.

(Idaho National Engineering Laboratory, S. Jones)

6. Soot Formation at Elevated Pressures Studied Using Laser Probe

Using advanced laser diagnostic techniques, considerable advances are being made in understanding the complex phenomena involved in the behavior of flames. The formation of soot, the familiar particulate matter resulting from incomplete combustion, is not only a serious source of reduced efficiency during combustion, but a potential environmental hazard as well.

Although there have been extensive studies of soot formation in combustion systems, most investigations have been carried out at normal or atmospheric pressure, despite the fact that, in practice, soot formation is most often a problem in systems that operate at high pressure. Applying advanced laser techniques, direct evidence has been obtained that soot formation increases at high pressures, not because the particles become larger, but because there are more of them.

While flames at elevated pressure are similar to those at normal atmospheric pressure, they become more compact as pressure increases. It was found that, with increasing compactness of the flame under pressure, the number of soot particles formed increases considerably. The experimental evidence comes from the much greater reduction in intensity -- by a factor of about 400 -- of a laser beam as it passes through a soot laden flame at two and one-half atmospheres of pressure compared to a soot laden flame at normal atmospheric pressure. Particle size very much affects the scattering of the laser light, and the ability to distinguish between either larger particles or more particles being responsible for the reduced beam intensity is dependent on sophisticated scattering measurements and their interpretation.

This study is typical of those now permitted by the advanced techniques for combustion research available at the Combustion Research Facility and has produced some important insight into the fundamental mechanisms responsible for the increase in soot production with pressure. Results such as these will ultimately provide the understanding necessary to control soot production in practical combustion devices operating at elevated pressure.

(Sandia National Laboratories-Livermore, W. Flower, and Stanford University, T. Bowman)

7. Highly Accurate Method for Isotope Ratio Measurements Devised Using Selective Ionization

A new, highly-selective method for measuring isotope ratios has been developed. The method, termed resonance ionization mass spectrometry (RIMS), is uniquely suited to the measurement of isotope ratios in situations where interferences from other elements are present. These interferences arise in mass spectrometry because ions are separated and detected according to mass. The problem of different atoms with the same mass occurs in both the lanthanide rare earths (e.g., cerium, used in color TV tubes, and neodymium) and actinide elements (e.g., uranium and plutonium). Resonance ionization is very selective, producing ions of only one element at a time, thus removing interferences without resorting to chemical separations or artificial measurement conditions, which seriously impair precision.

Research thus far has focused on the system cerium:neodymium:samarium (Ce:Nd:Sm) because Nd is an important element in nuclear reactor fuel burn-up analysis. Interferences from Ce (mass 142) and Sm (masses 144, 148 and 150) must be eliminated in order to arrive at an accurate isotopic analysis of Nd.

A high-powered nitrogen laser and a dye laser are used to produce light pulses of the proper wavelength to ionize Nd selectively in the presence of Sm and Ce. The ions thus formed are mass analyzed in a mass spectrometer. By switching the spectrometer back and forth between two masses, an isotopic ratio can be measured. The results obtained for isotopic ratios of Nd and Sm can be compared to the results from ordinary mass spectrometry taken under the same conditions. Errors of several hundred percent have been reduced to 1-2% with the new measurements!

(Oak Ridge National Laboratory, Dr. D. Donohue, Dr. J. Young)

8. Shear Added as a Variable to Equation of State for Fluids at Very High Flow

It has been found by techniques of molecular dynamics that in fluids, under conditions of very high flow, the equation of state includes a term involving shear as a parameter along with the usual variables of temperature, pressure and volume, necessary to define the intrinsic properties of a fluid.

Equations of state are used to predict the properties of fluids, including thermodynamic properties which are, in turn, used in the prediction of fluid behavior and the design of chemical processes. The discovery of the shear effect offers an explanation of previously unaccounted for observations of phase changes occurring under conditions of high shear. This discovery is expected to make it possible to predict thermophysical properties of complex fluids under conditions of unusual shear. Heretofore, there has been no awareness of the "shear" term because it makes essentially no contribution in the equation of state under normal conditions. Under conditions of very high flow or extreme mixing of a fluid, shear is high enough to have an effect.

The consequence of the shear effect is illustrated by the nitrogen-ethane system in which a region of non-miscibility, or a miscibility gap, is predicted by "normal" theory at given conditions of temperature and pressure, but disappears entirely when shear is taken into account. The nonexistence of a miscibility gap has significant practical consequences.

(National Bureau of Standards, H. J. M. Hanley - jointly supported by NBS)

9. The Effects of Mt. St. Helens and El Chichon Volcanos on the Stratosphere are Significantly Different

It is known that volcanic eruptions can change climate by injecting gas and dust into the stratosphere. Of the two components, volcanic dust usually has the shorter residence time in the stratosphere (up to several weeks) while the gas, consisting mainly of SO_2, is more gradually oxidized to sulfuric acid (H_2SO_4) and other sulfates that nucleate and grow to stratospheric aerosol particles capable of affecting the solar radiation balance of the earth.

The effects of the El Chichon, Mexico eruption of 1982 and the Mt. St. Helens activity of 1980 have been sorted out from solar radiation measurements taken with a computer-controlled radiometer developed at the Pacific Northwest Laboratory.

Although Mt. St. Helens produced a large spike of SO_2, its conversion to sulfate particles was rapid and the stratospheric aerosol injection was short-lived. Consequently, no long-term effect on weather is expected from stratospheric loading by St. Helens.

The pattern of aerosol development associated with the El Chichon eruption of April 1982 was quite different. Over middle northern latitudes, where the measurements were made, the first influx of stratospheric aerosol particles did not appear until September 1982, where an abundance of sub-micron sized particles was measured. The size of the particles has since grown steadily to approach a relatively large average diameter of one micron. The larger than expected size of the sulfuric acid particles and their long residence time may well change insolation and thus have climatological consequences.

(Pacific Northwest Laboratory, J. Michalsky)

10. Wear in Sliding Friction Shown to be Due to Surface Oxidation

A wide variety of systems have components such as clutches, brakes and commutator brushes where one surface slides over another with little or no lubrication. In such systems, different types of friction induced vibrations have been frequently observed. The squeal and chatter they produce can cause excessive wear of components, severe surface damage, and fatigue failure in addition to objectionable noise levels. Research on the underlying damage mechanisms has been focussed, in particular, on interactions between friction-induced vibration and wear.

Recent experiments have shown more clearly than ever before that mild wear is due to surface oxidation. Mild wear in this context refers to wear over the range of speeds and loads normal for use of sliding contacts between metals in dry (i.e., unlubricated) conditions. The experiments showed that formation of wear particles in mild wear is localized in the oxide film formed on the surface and is due to a fatigue mechanism. Further, mild wear was shown to be a function of the system rigidity that determines the frequency of slider oscillation and, hence, the number of loading cycles. The experiments also defined the conditions leading to the transition from mild wear to severe wear.

(Illinois Institute of Technology, S. Kalpakjian)

11. Tumor Forming Gene Eliminated in Widely Used DNA Vector in Plants

One of the impediments to "genetic engineering" in higher plants has been the lack of a suitable vector (a vector is an agent that can "carry" the desired gene) for transferring desirable genes into target plants. The candidate vector most studied has been a plasmid (DNA segment) deriving from the bacterium *Agrobacterium tumefaciens*. The plasmid (Ti) may be used to transfer pieces of DNA carrying specific genes into host plants. Several problems exist in using this vector, however one of these is having the genetic message carried by the Ti plasmid into the host expressed in the host, i.e., having the genetic message translated into a protein in the host possessing the ability to catalyze specific chemical reactions. Another is that the plasmid itself when introduced into the host plant causes tumors to develop in the plant.

Within the past year work has progressed to the point where it is now feasible by genetically altering the Ti plasmid and its introduced genetic message to eliminate tumor formation (called "disarming" the plasmid). Furthermore it is also possible to demonstrate the expression of an introduced genetic character in host plant cells. Three laboratories, two in the U.S. and one in Europe, conducted these experiments, to "disarm" the Ti plasmid and to demonstrate the new genetic character, independently and obtained similar results. This information brings the day closer to when it should be possible to introduce desirable traits into recipient plants with the objective of improving cultivated species.

(Washington University, M. D. Chilton)

12. Uranium Proven Unreliable Substitute for Transuranic Elements in Simulated Nuclear Waste Glass Studies

A study of simulated radioactive waste glass forms using uranium to substitute for transuranic elements has shown that they do not provide a reliable simulation of the structure and bonding properties of transuranics in silicate glasses. Since the leaching properties are dependent on bonding, this result indicates real waste systems must be investigated for reliable prediction.

To investigate the leaching behavior of radioactive waste forms, it is a common practice to study nonradioactive uranium analogs in order to simplify experimental procedures. For glass forms, air melted uranium glasses are generally studied which contain U^{6+} ions only. The assumption is made that the transuranic glasses will behave much like the uranium analogs. However, this procedure appears to be highly suspect, since transuranic glasses exhibit properties that are more similar to U^{4+} than U^{6+} glasses, and the results of EXAFS and X-ray photoemission experiments, and complementary investigations of the solubility and other phyhsical and chemical properties, have shown very different bonding characteristics of U^{4+} and U^{6+} ions in glasses. The important practical consequence of this research is that it demonstrates the unreliability of the usual simulation investigations of leaching in aqueous environments, where air melted glasses containing U^{6+} ions are used to simulate the same glasses containing transuranic elements

(Argonne National Laboratory, D. Lam)

13. Scientific Method Established for Assessing Hydrogen Donor Capacity of Solvents for Coal Liquefaction

A new procedure has been developed to assess how effective various solvents might be as sources of hydrogen in coal liquefaction. Liquefaction of coal involves breaking chemical bonds between carbon atoms and increasing the hydrogen content to establish more liquid-like properties in the system.

Since well established chemical principles involving bond dissociation energies form the basis of the new procedure, it can be used reliably to guide the production of better hydrogen donor solvents.

In this new procedure, a reactive chemical fragment, the orthoallylbenzyl radical, is generated by thermally decomposing the chemical substance orthoallylazotoluene. In the presence of a hydrogen donor or coal liquefaction solvent, this radical can either abstract hydrogen from the donor solvent or undergo an intramolecular rearrangement reaction. The two processes form two very different hydrocarbon products. Measurement of the yield or concentration ratio of these two products allows direct comparisons to be made of the hydrogendonor capacity of potential coal liquefaction solvents: the greater the yield of the chemical resulting from hydrogen abstraction, the better the donor capacity of the solvent.

The hydrogen donors studied thus far show expected trends of greatly increased rates of abstraction as the bond dissociation energy of the donor compound drops. The method is currently being applied to a wide variety of donor molecules and is ideal for the characterization of hydrogen donor solvent quality.

(Pacific Northwest Laboratory, J. A. Franz & Coworkers)

14. New Superconducting Shielding Method Reduces Magnetic Fields to Extremely Low Level

A new superconducting magnetic shielding method capable of reducing ambient magnetic fields to the nanogauss level has been demonstrated. This technique has the potential to revolutionize the methods of obtaining low and stable magnetic field environments necessary for low-noise operation of sensitive superconducting devices such as the Josephson Junction computer.

The method can be used to suppress magnetic fields to less than 10^{-10} Tesla, about one-half of one-millionth of the average magnetic field on the surface of the earth. This method can suppress magnetic fields more reliably and to lower values than any known technique. A very important utilization would be the shielding of such devices as computers which use superconducting elements from magnetic fields. During the necessary cooling down to operating temperatures near 4.2° Kelvin, any magnetic field may cause the sensitive superconducting circuit elements to malfunction.

This technique uses superconducting materials and some of their less obvious properties to remove and shield a region of space from magnetic fields. Superconductors exhibit the Meissner Effect: as a material is cooled below its superconducting temperature, it will expel the magnetic field. However, if the material is not a simple pure superconductor - and most practical materials are not - there will be "pinning sites" where some magnetic flux is trapped. Nearly twenty years ago, magnetic fields were shown to be quantized in units of about $2x10^{-11}$ Tesla. Thus each pinning site will trap an integral number of flux units. However, if a sufficient electrical current is passed through the superconductor, more than the "critical depinning current," the flux quanta become depinned and can be swept to the edge of the superconducting material.

This new superconducting magnetic shielding technique utilizes these fundamental properties to sweep the magnetic flux quanta from a long cylinder of a superconducting metal and thereby produce and maintain a region of space at the center of the cylinder at low or no magnetic field.

(Ames Laboratory, J. Clem)

15. First Measurement Made of Metallic Vapor Pressure of Einsteinium

The first measurement of the metallic vapor pressure of the man-made element number 99, einsteinium, has been made using material produced and prepared in the High Flux Isotope Reactor and Transuranium Processing Plant at the Oak Ridge National Laboratory. This is the heaviest and also highest atomic number element for which this fundamental thermodynamic measurement has been made. From the experimental data the investigators have derived a value of 31.2 kilocalories per gram-molecular weight for the energy required to vaporize the metal from a solid to a gas. This information is valuable for the increase in our understanding of the fundamental chemical and physical properties of elements and of their behavior in chemical reactions.

The measurements indicate that Einsteinium is a divalent metal, like calcium and magnesium, and thus quite unlike the lighter actinide element metals. This confirms earlier predictions based on the observed trend in the higher actinides, of the increasing stability of the divalent as compared to the trivalent state.

Einsteinium may well be the last element in the Periodic Table for which this type of measurement can be made because the next higher element, fermium, can thus far only be produced in hundred-million-fold smaller quantities.

(Los Alamos National Laboratory, J. Ward, and Oak Ridge National Laboratory R. Haire)

16. New Downhole Probe Measures Fluid and Heat Flow Simultaneously

As drilling for scientific purposes and for energy and material exploitation penetrates into rocks of increasingly hostile and variable properties, it is necessary to develop downhole measuring tools with enhanced capabilities. The measurement of heat flow in holes drilled through permeable rocks containing fluids can be a problem because it is difficult to sort out convective effects due to fluid flow from the effect of heat conduction through the rock itself. A research team focusing on new in situ downhole geophysical measuring techniques has developed an instrument capable of measuring and distinguishing between these two heat flow mechanisms.

The method depends on using a controlled heat source lowered into the hole to disturb the ambient heat flow regime in a reproducible way. In addition to a heat source, the instrument also has an array of temperature measuring devices (thermistors) that monitor the response of the natural environment to the artificially induced perturbation.

The response is fundamentally different for a convecting fluid system than it is for an exclusively solid rock conductor. A full three-dimensional analysis of the thermal perturbation problem allows calculation of the local fluid velocity vector and a good resolution between convective and conductive heat flow. The new probe has been successfully tested recently under field conditions at Long Valley, California, a thermally active potential target area for the Continental Scientific Drilling Program.

(Sandia National Laboratory at Albuquerque, J. Dunn)

17. Neutron "Time-of-Flight" Techniques Measure Residual Stresses in Structural Materials

Neutron "time-of-flight" techniques have been used to successfully measure residual stresses in cermet materials and in a zirconium alloy. The information on cermet materials is important in the design and development of drilling inserts for oil and gas well drilling apparatus. The detailed information on residual stresses in the zirconium alloy provides valuable data for reactor fuel element and pressure tube design and performance analysis. This new non-destructive method for measuring internal residual stresses in structural alloys was developed using neutron time-of-flight measurements and its success depends critically on the high resolution powder diffractometer located at the Intense Pulsed Neutron Source at Argonne. The technique was first applied to examine the zirconium alloy tubing used as fuel cladding in water reactors. It was demonstrated that it suffers from residual tensile stresses in the circumferential direction and compression through the thickness; this combination can lead to unexpected and unacceptable creep of the cladding in service. The second application was to measure the stress level in the metallic binder phase of a hard ceramic-metal composite used as drill bit inserts for rock drilling; the high tensile residual stress found can cause premature failure of the drill bit.

This research has developed and applied a non-destructive method for characterizing quantitatively internal residual stresses. No other probe has been successful in achieving this, with the possible exception of an acoustic technique. This research will impact technically on the processing of structural materials, namely, to change these to reduce unwanted stresses and enhance desired ones. The potential economic impact is large in terms of allowing improved reactor fuel utilization in the case of the zirconium alloy and longer drill-bit life in the case of the composite noted above.

(Argonne National Laboratory, J. Faber, in collaboration with Chalk River Nuclear Laboratory, Canada,

18. Helium Atoms Found to Create Lattice Defects in Metals

A new physical process by which an impurity (helium) can produce lattice damage in metals in the absence of externally-supplied energy (i.e., thermal, radiation) has been verified experimentally. It has been known for some time that helium atoms are readily trapped in metals that have large numbers of defects in their lattice structure, e.g., as in damaged metals. More recent research has shown that helium atoms also become strongly trapped in metals with low intrinsic defect concentrations. These results stimulated calculation of lattice defects to account for the observations and have led to a model involving self-trapping of the helium. This theoretical work was followed by microscopic verification of helium-induced bubble formation in tritium charged palladium and in gold where helium was implanted at energies below the threshold that would normally cause lattice damage. In addition, evidence of helium-induced bubble formation has been found in vanadium and niobium. These latest studies have yielded new data on bubble growth processes and helium-dislocation interactions.

Thus the process of helium self-trapping in metals whereby helium forms its own lattice defects which nucleate helium gas bubbles was first indirectly inferred from experiment, then predicted by theory, and finally experimentally confirmed for four different metals and metal hydrides.

These results alter present thinking on the role radiation damage plays in helium bubble formation in metals and have shown that helium-induced degradation of metals cannot be ruled out as a potential problem area in long-term fusion energy applications. They also call attention to the possibility of future materials problems in all nuclear-based technologies. These results are directly applicable to other ongoing modelling studies of material response in fission reactor environments.

(Sandia National Laboratories-Livermore, W. D. Wilson, G. J. Thomas, and M. I. Baskes)

19. New Method to Uniformly Blend Ceramic Powders With Sintering Additives Improves Properties

A new method was developed for the homogeneous addition of sintering aids to silicon nitride powders. Sub-micron sized silicon nitride powder, when sintered, or heated under defined conditions, becomes a high-temperature structural ceramic. Sintering aids promote this process. Homogeneity of the unsintered compacts is an essential requirement in order to properly sinter silicon nitride to obtain uniform, reliable, ceramic components. The method developed is based based on the use of colloidal dispersion forces, first, to break down and prevent the formation of agglomerates in unsintered compacts of silicon nitride powder, and second, to promote mixing by causing uniform dispersion of sub-micron powder mixtures of silicon nitride and the sintering aids yttrium oxide and magnesium oxide.

A comparison of the mixing achieved by this new process with that achieved by conventional powder processing routes showed that this new method provided a dramatic improvement in the uniformity of silicon nitride unsintered compacts.

Homogeneity of the unsintered compacts containing silicon nitride and its sintering aids is necessary to produce a homogeneous flaw-free microstructure by the sintering process. Such a microstructure is required if the silicon nitride is to have good mechanical properties at 1500°C, such as for potential use in advanced turbine blades.

(Rockwell International Science Center, F. F. Lange and T. M. Shaw)

20. New Method Devised for Monitoring Thermally Enhanced Oil Recovery

The velocity and attenuation of seismic waves traveling through rocks is strongly influenced by the properties and spatial distribution of the pore fluids present. An investigation of these phenomena and their relation to bulk rock properties, pore distribution in the rock, and the presence and nature of the pore fluid, has led to a new method for reliable remote monitoring of the progress of steam flooding and other oil recovery methods. The advance results from the ability to follow changing oil temperature throughout the process. While measuring the velocity and amplitude of seismic signals as a function of pressure (up to 200 bars) and temperature (up to 150° degrees C), very large reductions in velocity (50%) and wave amplitude (7 fold) were detected when heavy-oil saturated sandstones were heated under in situ pressure conditions.

Making use of this effect, an array of seismic receivers and transmitters deployed over an oil reservoir can be used to monitor the progress of a thermal oil recovery operation. The array measures the variation of seismic velocities and amplitudes during the recovery operation, and these data can, in turn, be used to model changing oil temperature throughout the reservoir.

(Stanford University, A. Nur)

21. Improved Method Developed to Describe Crack Strain Fields in Heavy Piping and Pressure Vessels

An effective computational method was developed which permits far more realistic properties of materials to be employed in the design of major components of energy plants than allowed by current design codes. The new method which is a finite element technique, treats the deformation behavior of metals in a manner termed "incompressible-fully plastic." Though still an approximation, this is far superior to previous descriptions of strain fields around cracks in piping and pressure vessel alloys where the materials were treated as "linear elastic."

With the new finite element technique, engineering calculations of the stability of a crack have been carried out under the auspices of the Electric Power Research Institute. It recently published a handbook as a reference source for solution of crack stability problems in piping and pressure vessels, which acknowledges that the calculations were made possible by the development of this finite element technique.

By providing a computational method for accurate failure analysis, this research has paved the way for proposing improved design criteria for qualifying structural components in nuclear reactors with lower initial cost than with current codes. The improved design criteria will also assist in qualifying components for continued service; the economic value of this is significant as well, given given the current trend toward extending utilization of existing plants rather than building new ones.

(Brown University, R. Asaro, J. Gurland, and A. Needleman)

22. Miniaturized Thermionic Elements Introduced into Integrated Circuits

Measurements of temperature, pressure, mass flow rates and the like often have to be carried out in an environment in which the usual instrumentation fails. Devices using semiconductors, for example, cannot be employed at temperatures above a few hundred degrees. On the other hand, devices using electron emitting elements (as in the triodes of vacuum tubes) can in principle operate well in a variety of hostile environments, but until now no way had been found to incorporate such elements in integrated circuits comparable to semiconductor microcircuits.

Recently a promising step toward solving these problems has been completed. Extremely small thermionic elements have been devised and shown to be well adapted to fabrication and use in microcircuits etched on silicon chips. Packing densities of 1000 circuit elements per square inch have been achieved and outstanding tolerance of high temperatures and radiation levels has been demonstrated. The present state of this art is not yet at its limits and further important advances are anticipated.

Unexpectedly, early results from this research have attracted the attention of a major computer products manufacturer and are being applied by that manufacturer to computer terminal display tubes. The tubes will feature an electron gun with multiple sources and built-in capability for signal processing. Although this application was not foreseen, a broad range of applications of the new integrated thermionic circuit technology is expected in the long run for instruments of interest to DOE energy and defense programs.

(Los Alamos National Laboratory, B. McCormick)

23. Unexpectedly Fast Electron Transfer Across Large Molecules Discovered

A novel set of experiments has demonstrated that electrons move surprisingly fast across large molecules. The molecules were designed with a rigid bridge separating parts of the molecule that can accept electrons at fixed, known distances. In the experiment electrons generated in a linear accelerator attach themselves at one end of each molecule and the rate at which they move to the other end is measured. Because the measured rates are extremely fast, and the spacer region is an electron insulator, it was determined electron transfer was accomplished by a "tunneling" or jumping mechanism. These results are of particular importance in the solar photochemistry research area where initial charge separation following absorption of light energy may be accomplished following such a jump.

(Argonne National Laboratory, J. Miller)

24. Neutron Reaction Cross Sections Extended By New Technique

High resolution measurements of neutron and gamma ray production cross sections have been made for the first time for neutron bombardment energies above 15 MeV. These measurements were made simultaneously over the range from 200 keV to 40 MeV using the intense pulsed beam time-of-flight system at the Oak Ridge Electron Linear Accelerator (ORELA) and were made possible by a new technique based on a high resolution lithium-doped germanium detector. Although these cross sections are of primary interest to the Office of Fusion Energy, the initial measurement provided information of timely importance to the fast reactor program, clearing up a troublesome descrepancy between experimental and theoretical results for an important design benchmark, the "large iron sphere". The measurement of the isotope iron-57 demonstrated that this minor component of natural iron (2.2% abundance) can not be ignored in the calculation. The observation of a surprisingly intense gamma-ray line, the measurement of which was made possible by the high resolution detector used, also has provided valuable information for the theorists who are developing a complicated nuclear model for the calculation of these cross sections.

The cross sections being measured with the new system are of interest not only for direct input into calculations of neutron transport and activation, but are also contributing to the development of a computational model that will permit the prediction of cross sections for high energy neutron reactions that are difficult or time-consuming to measure, but are needed for inclusion in the Evaluated Nuclear Data File (ENDF) maintained by DOE.

(Oak Ridge National Laboratory, D. Larson)

25. Elusive Energy Loss Process Affecting Fusion Verified

Measurements of dielectronic recombination, a process that has eluded experimenters for years, have finally been made. The dielectronic recombination cross sections for the doubly charged ion of boron were measured; that is the first time such measurements have been made for an ion with multiple charges

Dielectronic recombination involves the loss of energy in a plasma and occurs when energy is absorbed by an ion when it captures an electron in the plasma. At the instant of capture, the positive charge on the ion is reduced by one unit and the resulting ion is left with excess energy. The ion next rids itself of the extra energy by the release of a photon most likely in the form of an x-ray. The net effect of all this is that the energy initially provided to effect a collision between two atoms and cause fusion of the two nuclei is instead lost through radiation. The process is important to the understanding of the behavior of plasmas and its measurement helps provide a more accurate account of the energy balance in a fusion plasma. This account in turn will permit the improved design of efficient fusion power plants.

The existence of the process was first suggested in the 1940's to account for observations made by astrophysicists to explain energy balance in stars. They could only observe the sum of several simultaneous processes, of which dielectronic recombination was one. Experimental study of the single isolated process was not possible. Now the process has been demonstrated by directing a beam of ions from an accelerator into a specially designed chamber filled with electrons. Close inspection of the interaction taking place in the chamber between the ions and electrons showed the effect sought.

While the first results are in some disagreement with theory, the fact that the process can now be studied experimentally is clearly a breakthrough in the field of high energy atomic physics and a significant contribution to our improved understanding of fusion plasma interactions.

(Oak Ridge National Laboratory, S. Datz, & co-workers)

26. Transposition of Genes in Higher Organisms Quantified for the First Time

Only recently has it been appreciated that genetic transposition (movable genes) does occur in a broad range of organisms. This phemonenon, which was discovered in maize by Dr. Barbara McClintock about thirty years ago, has never been quantified as to its rate of occurrence.

In a specially designed genetic system in maize the frequency of transposition of genes associated with the restoration of male fertility has been measured. This represents the first time that these events of movement of genes have been put on a numerical basis. Such results will assist in assessing the importance of genetic transposition and in understanding the phenomenon itself.

(University of Illinois, J. Laughnan)

27. New Method for Numerical Solution of Turbulent Combustion Model

Difficult questions in computational mathematics arising from the need to simulate real problems are being examined. One such question is a fundamental and complex problem in the area of turbulent combustion: the analysis of the effect of turbulence on the propagation of a flame. At high Reynolds number, turbulent eddies and recirculation zones form due to viscous effects. This affects the position of the flame and the distribution of unburnt fuel available for combustion. This interaction is of great importance in the design of internal combustion engines. The problem is to discover how to direct the flow in such a way that the largest amount of fuel is burned as quickly as possible, thus maximizing the force on the piston and minimizing the amount of unburnt fuel expelled at the end of a stoke.

To investigate these phenomena, a numerical technique was developed to approximate the solution of a mathematical model of turbulent combustion. This technique is specifically designed for flow at high Reynolds numbers. It portrays in a natural and effective manner the development of turbulent eddies and recirculation zones in the flow. The motion of the flame is handled in a manner that avoids the instabilities and inaccuracies that plague other front tracking techniques. The results of "numerical" experiments with this new technique on turbulent combustion in open and closed chambers show the effect of heat-producing reactions and viscosity on the rate of combustion. Heating effects along the front are seen to increase the speed at which the flame travels through the domain, decreasing the amount of time required for complete conversion of reactants to products. Viscous effects, on the other hand, both retard and accelerate flame advancement. Although the turbulent eddies produced by boundary conditions inhibit burning in corners and near walls, they also "wrinkle" the flame, increasing the surface area available for combustion. These "numerical" experiments represent a major step towards understanding the combustion process.

(Lawrence Berkeley Laboratory, J. Sethian, A. Chorin)

28. Unexpected Photochemical Mechanism Discovered in Enzyme Process for Biomass Hydrogen Production

A new photochemical route to the utilization of photons for enzymatic dissociation of water to produce hydrogen from biomass has been discovered. Experimental measurements of the simultaneous generation of hydrogen and oxygen by a laser light saturation technique have established the unexpected insight that not all photodissociation of water occurs by the same photochemical mechanism. By examining the hydrogen to oxygen ratio, it was apparent that the rate of hydrogen and oxygen generation was inconsistent with the time-accepted Z-scheme mechanism of photosynthesis. The hydrogen to oxygen ratio was found to be significantly below the 2:1 ratio of water's composition, which suggested the existence of a chemical step that encumbers the release of hydrogen. The fact that a previously unexpected mechanism exists for the enzymatic dissociation of water in biomass systems has broad implications for future developments in solar photochemistry as well as in the case of biomass photolysis.

(Oak Ridge National Laboratory, E. Greenbaum)

29. Physics Model Computations Nearly Ten Times Faster Using New Computer With Parallel Architecture

Techniques for accelerating execution of practical computational problems by using parallel processing techniques on an experimental computer have been successfully demonstrated. In mid-1983, a Denelcor HEP-1 computer was acquired as part of the DOE activity in experimental parallel architecture research.

Three problems common to the DOE activities in computational modeling were addressed: a particle-in-cell model, commonly used in plasma physics models; a hydrodynamics model, used in weapons design and combustion modeling; and a Monte Carlo model, used in modeling critical phenomena in materials and in fundamental particle physics. In each case, the problem was studied with the aim of redesigning the algorithms into sets of independent processes that could be executed concurrently. The HEP-1 architecture provides a mechanism for simultaneously executing a large number of independent processes, thereby speeding up the computation by a factor proportional to the number of processes. It was demonstrated that the computations involved in each of these modeling problems could be carried out about ten times facter with this architecture.

These results hold great promise for the design of even faster parallel architecture computers for large scale scientific computation.

(Los Alamos National Laboratory, B. Buzbee)

30. Genes Controlling the Primary Events of Photosynthesis Identified

Using molecular genetic techniques scientists have succeeded in cloning and sequencing of the nucleic acids of five genes which code for some of the first steps in photosynthesis. This work represents the first time that it has been possible to precisely locate specific genes that code for proteins involved in the primary events of photosynthesis in a structure known as a reaction center and the related "light harvesting" pigment area. This work was done with the photosynthetic bacterium known as Rhodopseudomonas capsulata; however, similar genes are operative in higher plants. Further, the region of common function in this genetic material has been conserved over three billion years, the estimated evolutionary time between the bacteria and higher plants.

The significance of the work is that it permits more incisive questions to be asked about the structure and function of the biological energy conversion entity known as the photosynthetic apparatus. For example, the information on the nucleic acid sequences is easily translated in amino acid sequences in the photosynthetic proteins. That information has led to clues about how some of the components of electron transport (quinones) are attached to the proteins.

In addition, some of the proteins also have homology with those that are involved in the action of some widely used herbicides in crop production. Thus such information may also provide leads into understanding of herbicide action and possible strategy for better molecular designs of herbicides.

(Lawrence Berkeley Laboratory, J. Hearst, and K. Sauer)

31. New Techniques Developed for Analyzing Near-Surface Reactions

Two new techniques, one involving electron and photon desorption, and the other pulsed laser field evaporation have provided the means to substantially advance the understanding of atomic and molecular motion in the near surface regions of solids.

Photon stimulated desorption studies of cleaned silicon surfaces revealed that hydrogen migrating from the bulk to the surface displays a complex surface reaction resulting in the formation of hydride phases. These studies are important not only for the determination of bonding site, electronic state, and geometric configuration, but also to the technological goal of removing hydrogen from silicon.

Pulsed laser studies have shown that surface crystallography plays a major role in the catalytically important process of molecular dissociation. The temperature range over which carbon monoxide molecules dissociate has been measured, as has, for the first time, the activation energy between flat and stepped regions on the surfaces of molybdenum. These experiments showed that highly-charged field-evaporated ions are formed away from the surface after the atom has desorbed to a lower charge state.

The advances in both of the techniques will permit new insight into surface and near-surface reactions which are important to a number of technological areas.

(Sandia National Laboratory - Albuquerque, M. Knotek and G. Kellogg)

32. Dose Dependence for Defect Production Mechanism Found Using ANL High Voltage Electron Microscope (HVEM)

The unique capabilities of the Argonne National Laboratory High Voltage Electron Microscope/Tandem van de Graaff have recently been employed in attacking a controversial issue involving the nature of defects formed in the alpha-phase of iron during neutron irradiation. The basic character of the defect structure produced during neutron irradiation was reproduced by ion bonbardment and examined in situ at 40°K in the ANL-HVEM. The defect formation mechanism observed differs from what had been assumed previously, and is different from that for most other metals. It was found that the defect producing mechanism caused by high energy knock-ons (in either ion or fast neutron irradiation) changes when the dose is high enough. This research, uniquely dependent on the ANL-HVEM capability, is the first demonstration of a dose dependent change in a defect production mechanism. It will have to be included in valid models of irradiation behavior in the future and could have important consequences for predictions of radiation damage in iron and ferritic alloys. The low swelling character of these materials may, in part, be related to this newly discovered effect.

(Argonne National Laboratory, M. Kirk, and University of Illionis, I. Robertson)