Some Examples of Accomplishments Under the

Basic Energy Sciences Program During 1981

While these selections may not reflect the full range of the basic research carried out through more than 1000 projects supported by Basic Energy Sciences, they are examples of how basic research can be brought to bear to resolve a variety of energy problems.

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1. New Measurement of Californium-252 Neutron Yield Standard

The spontaneous fission of californium-252 is used as a standard against which measurements of the interaction of neutrons with nuclei, from any source, including other fissioning isotopes (e.g., uranium-235 and plutonium-239), are made. A significant nuclear data effort has produced a new and definitive measurement of the average number of neutrons emitted per fission (a parameter called nubar, $\bar{\nu}$) for californium-252. This experimental program, carried out over a period of five years, has resulted in an unprecedented accuracy for this type of measurement. The uncertainty assigned to the new value of $\bar{\nu}$ is less than 0.2%. Achieving this accuracy involved painstaking experiments and exhaustive analysis of possible experimental errors. This new measurement, besides its fundamental importance in neutron physics research, has immediate impact on fuel cycle costs in light water reactors. The fission fuel consumption rate in reactors depends strongly on the value of $\bar{\nu}$ and more cost effective scheduling of fuel cycles and fuel enrichment can be achieved if $\bar{\nu}$ is known to very high accuracy. It has been estimated that savings of $250,000 per fuel cycle per reactor can be realized solely on the basis of the improved accuracy resulting from this work. Economies in designing fast breeder reactors should also be realized. The californium-252 used in these experiments was produced at the High Flux Isotope Reactor (HFIR) at Oak Ridge.

(Oak Ridge National Laboratory, R. Spencer, R. Gwin, and R.Ingle)

2. Theoretical Prediction of Solid State Physical Properties

As a result of recent theoretical investigations, it is now possible to calculate many structural and vibrational properties of solids using only fundamental properties of constituent atoms as input. These calculations give results within 5% of measured data for silicon and germanium and include values for the following fundamental critical parameters: lattice constants, cohesive energy, bulk modulus, shear modulus, and phonon structure. These parameters determine other macroscopic engineering properties such as strength and thermal conductivity. In addition, the studies showed, for the first time, that the temperature and pressure of solid phase transitions could also be calculated. The computations made possible by this theory are significant for conducting research on photovoltaic solar materials, catalytic properties of surfaces, and for predicting the strength and thermal stability of materials. In addition, the theory holds promise for making accurate calculations of superconducting properties important to fusion, for example, from theoretical knowledge of the interactions of electrons and phonons. This is an important step along the way to enabling the design of new materials that are tailor made for particular applications.

(Lawrence Berkeley Laboratory, M. Cohen)

3. New Non-Destructive Downhole Seismic Source

A new downhole seismic source developed for magma exploration has enhanced our ability to define underground structures. It offers a new capability for delineating underground oil and mineral resources, and has attracted interest from oil company exploration geophysicists. The new method devised as part of a study of the energy potential of buried molten rock, employs a pneumatically-driven vibrator that operates deep within a borehole. The vibrator generates a single frequency seismic wave-train 10-seconds long. The waves travel through the surrounding formation and are received by an extensive array of surface geophones. Downhole excitation sources have always been attractive because of the direct path geometry to the geophone detectors array. The result is that ample seismic energy for convenient, reliable data collection is delivered to the formation without significant damage to the borehole. Previous downhole sources, which have been either explosives that damage the hole, or one-shot mechanical pulsers, do not enable repetitive data collection. The new approach can further be tailored to concentrate its energy into either compressional or shear waves of a desired frequency for extended duration. These different types of waves can be used to distinguish between solids and liquids. The new method has been successfully applied for its original purpose, providing measurements of seismic wave transmission through hot hydrothermal zones above partially molten rock. A new version of the seismic source, now under construction, will be compatible with standard logging cable and will have a variable frequency capability for use with more powerful sophisticated signal analysis techniques.

(Sandia-Albuquerque, H. Hardee and U. of Texas, R. Ward)

4. Basic Science Applied to Fabrication of Corrosion Resistant Intermetallic Materials

The commercial potential of a major class of materials called intermetallics was increased considerably with the development of a new fabrication technique. This was made possible from better understanding of the properties and structure of intermetallic compounds. These have ordered atomic configurations in contrast to disordered atomic configurations in metallic alloys. Because of this structural characteristic, intermetallic compounds have distinct advantages over alloys, including chemical and mechanical stability. Yet, because of their structure, intermetallics are difficult to deform without fracture.

The intermetallic Fe_3Si commercially is cast into thick wall corrosion-resistant pipe for the chemical industry where weight is not an important design consideration. Heretofore, it was not possible to produce thin wall tubing; this would require extrusion, and the Fe_3Si structure does not exhibit sufficient plasticity to avoid cracking during hot extrusion. By starting with a modified composition that could be extruded, it was found that the desired intermetallic compound could be produced through a phase change subsequent to the extrusion step; the resulting product thus has both the desired form and properties. Steel tubing clad with

Fe_3Si has greater resistance to cracking under tensile loads and it was produced for the first time using conventional metal working techniques. This achievement represents a significant first step toward fabrication of thin gauge Fe_3Si intermetallic compound products for automotive and other industrial applications.

(Ames Laboratory, F. Kayser)

5. Laser Based Technique Permits Study of Critical Trace Species in Flames

Saturated absorption spectroscopy, a new laser-based technique is being used to study some of the less well understood aspects of combustion. A flame can be scanned to measure the location and concentration of highly dilute chemical species that are difficult, if not impossible, to detect by other means. This new technique holds promise for identifying and understanding the roles of dilute, but highly reactive species believed to be important in combustion. The technique uses crossed laser beams, to define a small volume element (essentially a point) within the flame. One beam is much more intense than the other. At a proper choice of wavelength the intense beam excites a large fraction of the species under study to an energy level characteristic of that species. The second beam, of the same wavelength, is much lower in intensity. If one measures absorption of the second beam when the first beam is off and then on, one finds a decrease which is proportional to the number of molecules excited by the first laser beam. Since the number of molecules excited is, in turn, proportional to the total number present, their absolute concentration can be determined after the process has been suitably calibrated.

(Sandia National Laboratory, Livermore, J. Goldsmith)

6. Predictive Model for the Ductile-Brittle-Tranaition-Temperature for Ferritic Steels

A major step was made toward quantitative prediction of the ductile-brittle-transition-temperature (DBTT) in ferritic steels. The DBTT is one of the least understood, yet one of the most important mechanical properties of steel. Above the DBTT, steel is tough; below, it is brittle. A semi-empirical model that incorporates both the theory of alloys and applied mechanics has been shown to have quantitative validity for binary iron alloys. It can account for the effect of different solute concentrations in these alloys on the DBTT. This is a significant first step toward understanding and controlling a property that has puzzled scientists for years. This model may lead to a capability to predict as well as explain radiation induced changes in the DBTT which now must be experimentally verified with in-reactor test coupons to assure the integrity of nuclear reactor pressure vessels.

(University of Minnesota, W. Gerberich)

7. <u>New Process to Recover Uranium from Leach Liquors</u>

A new process to recover mined uranium from *in-situ* leach liquors has been developed. The new process, utilizes hydrogen peroxide. It replaces the current batch process using ammonium hydroxide, which has been virtually prohibited by EPA restrictions. These restrictions relate to the hazards to humans of ammonia ingestion from large-scale operations. The new hydrogen peroxide process is continuous and is characterized by faster filtration rates, improved separation of the uranium from contaminating metal elements such as molybdenum and vanadium, and culminates in a crystalline form of uranium peroxide particles with a narrow size distribution and low concentrations of impurities. The process is important not only for faster recovery rates, but also for its efficiency in removal of molybdenum and vanadium which adversely affect the properties of the processed uranium as a nuclear fuel. The process evolved from interaction among scientists and engineers in several different areas. When researchers knowledgeable in the surface sciences were made aware of the uranium recovery problem they devised this innovative solution to it.

(Ames Laboratory, L. Burkhart)

8. <u>Highly Specific Extractants Synthesized for Recovery and Purification of Valuable Metals</u>

Research started in 1980 has led to the discovery of bifunctional extractants for recovery and purification of actinides from nitric acid and from other nuclear waste solutions. They also can be used for recovery of certain valuable fission products, e.g. palladium, from high level liquid waste. This new class of bifunctional extractants, i.e. extractants which have two potential donor groups in the same molecule, are called carbamoylmethylphosphine oxides (CMPO). The carbamoyl and phosphine groups are connected by a methyl (CH_2) group. The nitrogen of the carbamoyl group has two organic groups attached to it as does the phosphorus in the phosphine group. By proper choice of these two sets of organic groupings it is possible to synthesize a CMPO which extracts americium from nitric acid solutions with a distribution coefficient greater than 20, that is, over 95% extraction efficiency. Tetra- and hexa-valent actinides are extracted with even higher distribution coefficients. Selectivity of actinides from practically all fission products is achieved by "scrubbing" with nitric acid-oxalic acid.

(Argonne National Laboratory, E. P. Horwitz)

9. New Photochemical Reaction for Producing Hydrogen

Sunlight, striking a photoelectrochemical cell containing a tungsten disulfide semiconductor electrode in a concentrated solution of sulfuric acid, will convert sulfur dioxide to sulfuric acid with the simultaneous formation of hydrogen. This photochemical reaction, which takes place with sunlight as the only energy source, occurs with 5% efficiency in normal sunlight and without degradation of the materials involved. This reaction is particularly interesting because of a known thermal reaction that decomposes sulfuric acid into sulfur dioxide and oxygen. The coupling of these two reactions would conserve sulfur dioxide and sulfuric acid; the result would be a reaction system using heat and sunlight to decompose water to hydrogen and oxygen without undesirable waste products. So far the reaction has been studied only with expensive single-crystal tungsten disulfide. Less expensive polycrystalline materials seem possible. The reaction of SO_2 to produce H_2SO_4 is also of considerable interest in the fertilizer industry.

(Massachusetts Institute of Technology, M. Wrighton)

10. Internal Friction in Car Tires - Model for Energy Loss Characteristics

A collaborative University-Industry research effort has led to the formulation of a preliminary theory of energy losses in car tires (rolling friction). In conjunction with concurrent experiments on various tire materials, this research holds promise for impressive energy savings in the transportation sector. For a long time automotive engineers have known that over 10% of the gasoline consumed in driving is lost to tires. The energy is dissipated through internal friction. Internal friction, produced as the tires flex in rolling, heats the tires, generally makes them weaker and produces no benefit. The present approach to tire design is largely a cut-and-try process with little regard to the mechanisms for energy consumption. One reason for this has been the absence of a good model for internal friction generated in composite materials such as reinforced rubber used to construct tires, V-belts or conveyor belts. The formulation of this model provides an initial essential step towards filling this major gap in our knowledge. The starting point of this research is the theory of viscoelastic composites, i.e., modelling of the actual heterogeneous medium by a homogeneous medium such that the properties of the latter approximate reasonably well the macroscopic properties of the actual composite. Typically, tires are made of such disparate materials as rubber which flexes, stretches but is not very compressible, and cord which stretches to a limited extent under tension, but which offers little resistance to bending or compression. Both materials dissipate energy differently as the applied stress changes. Recent results have contributed to an understanding of how to combine these properties into a single realistic model material which should be valid over a wide range of operating parameters. Thus, this theory together with the new experimental results on about 100 samples of tire materials will provide a means for predicting the internal rolling friction in a tire of a given design.

(University of Michigan, S. Clark; B. F. Goodrich Co., F. Tabaddor)

11. Microbial Synthesis of Larger Molecules from Carbon Monoxide

Methanogenic bacteria are a unique group of anaerobic organisms which have not been studied extensively. These bacteria are able to grow using carbon monoxide as a sole carbon and energy source. Recently a mutant of one bacterium in this group was found to be capable of converting carbon monoxide and other single carbon compounds to acetic acid. The significance of this discovery is that it may lead to a bioprocessing strategy for handling the unwanted gases produced in high temperature processing of biomass and coal. Such a scheme would have a two-fold advantage in disposing of waste products and at the same time producing materials which are valuable in the chemical industry. Other metabolic mutants of this organism are being isolated as an aid to understanding the pathways of metabolism involving single carbon compounds.

(University of Wisconsin, J. G. Zeikus)

12. Model to Predict the Effect of Residual Stress on Superconducting Materials

An analytical model that predicts the residual stress in superconductors has already helped fusion researchers to optimize design and fabrication of large superconducting magnets. Superconducting magnets can produce strong magnetic fields with little expenditure of energy. In general a larger supercurrent and stronger magnetic field can be obtained when the residual stress in the superconductor approaches zero. The model predicting residual stress requires only knowledge of the volume fraction of each component in the composite conductor where, for example, the superconductor is Nb_3Sn and the other components are Nb, Cu and Ta. Thus different proportions of components give different residual stresses, and the selection of materials for producing an optimum superconductor must consider minimizing the residual stress obtained for that choice of materials. This selection process can now be done analytically rather than by the past "cut and try" experimental approach.

(Oak Ridge National Laboratory, D. Kroger, C. Koch, D. Easton)

13. Irradiation Stability of Ceramics for Radioactive Waste Disposal

Materials used for storage of high level radioactive waste must be mechanically stable over geologic periods to insure that no hazardous material escapes into the biosphere. A relatively new concept for storage is the use of synthetic rock to sequester the most hazardous species. Synthetic rock is a man-made ceramic material modeled after minerals that are known to be stable for a very long time. An experimental program in cooperation with Australian scientists has been examining the resistance to radiation effects of a candidate mineral, hollandite, which is theoretically attractive for storing cesium, one of the most hazardous species. Hollandite was exposed to the equivalent of 1,000,000 years of radioactive decay in laboratory experiments using an accelerator. The experiments showed that hollandite did not crack or experience a significant volume change, thereby suggesting validity of the "synrock" concept. Other mineral structures known to exhibit long term geologic stability, and having atomic structures compatible with the longest lived components in radioactive waste, will be studied with the goal of developing a design methodology for synrock waste host materials from several compatible mineral phases.

(Battelle Pacific Northwest Laboratory, W. J. Weber)

14. Fracture in Ductile Metal Observed by Microscopy

Fracture in ductile metal is of great practical importance. This phenomenon was investigated under high resolution electron microscopy, and for the first time, fracture was photographed as it actually took place. Photographs of aluminum under tensile stress in the electron microscope were taken. The aluminum sample appeared to fracture as a result of two mechanisms, one involving stress, and the other failure in a dislocation-free zone. The latter observation is new. It offers insight into the understanding of the fracture of ductile metals, and will assist in the design of ductile alloys with higher resistance to fracture.

(Oak Ridge National Laboratory, S. M. Ohr)

15. Dynamics of Molecular Ions Now Accessible Through Controlled Coulombic Fragmentation

A new technique now permits the experimental determination of the structure and binding forces in molecular ions. These ions are extremely reactive species that can have profound effects on chemical reactions. This great reactivity has made it impossible to determine the structural and binding characteristics of molecular ions except in a few rare situation. The ion studied is accelerated and passed through a thin crystal, which gently strips electrons from the ions. This leaves constituent atoms positively charged, so that electrostatic repulsion breaks the ion apart. As the constituent charged atoms separate, the time and place of detection of these fragments are determined and can be used to calculate a series of "snapshots" of the ion as it disintegrates. This information in turn reveals the forces binding the atoms together in the ion. Among processes that can benefit from this knowledge are the direct conversion process in MHD and studies of energy loss mechanisms in fusion plasmas.

(Argonne National Laboratory, D. S. Gemmell, R. P. Kanter)

16. <u>Fluorescence of Actinides: Highly Sensitive Monitoring Technique</u>

Clever choices of laser excitation frequencies have enabled measurement of fluorescence spectra and lifetimes of actinides in aqueous solution. This may make possible routine monitoring of actinides in process chemistry and in the aquatic or geologic environment. Early studies of actinide emission spectra had indicated that the fluorescence spectrum and lifetime of curium species in the +3 valence state should be observable but not those of other +3 actinides. The curium (+3) fluorescence has now been measured in remarkably dilute concentrations of about 10^{-9} molar. Further detailed studies using carefully chosen laser excitation have now shown that similar observations are also possible for einsteinium (+3), and almost certainly for berkelium (+3) and americium (+3). These techniques are being extended to other valence states of the actinides so that similar information can be obtained for uranium, neptunium, and plutonium. Since the energy and lifetime of fluorescence radiation is highly sensitive to the identity of the actinide species and its valence state this information may lead to the development of powerful techniques for monitoring actinides.

(Argonne National Laboratory, J. Beitz)

17. <u>Change in Catalyst Substrate Dramatically Changes Fuel Product</u>

Preliminary experimental results have dramatically shown that the specificity of the catalytic conversion of coal synthesis gas ($CO + H_2$) to methanol and methane is dependent on the type of silica substrate used to support the palladium metal catalyst. Palladium on Grade-57 gel was almost 100% selective in catalyzing the formation of methanol whereas palladium on Grade-01 gel had 100% selectivity to methane. Palladium on Cab-O-Sil was found to produce both fuels. The significance of this discovery is knowledge that the ability of the palladium to catalyze the synthesis of methanol is <u>not</u> an inherent, general property of the metal alone. This is one of the most dramatic examples known of a substrate effect in heterogeneous catalysis. Research is in progress to explain this observation, which may strongly influence the use of synthesis gas from coal.

(Texas A & M, J. H. Lunsford)

18. Coal and Oil Shale Non-Destructively Analyzed for Organic Matter

Valuable samples of coal solutions and oil shales were subjected to rapid non-destructive tests based on small angle scattering of neutrons. One objective was to learn if this technique could be used to physically characterize the samples prior to other necessary, but destructive tests. Very useful results were obtained: the concentration of coal in solution could be measured over a dynamic range of 10 and the size and shape distribution of pores in oil shale determined. Contrary to earlier assumptions, it was learned that the pores did not flatten with increasing lithostatic pressure (depth). Indeed, there does not seem to be a clear correlation between pore size and depth which means that specific site-depth testing is required before deciding how to extract oil from oil shale on a large scale basis. The neutron technique is extremely efficient requiring only a few hours for a full analysis and can cover a wide range of solution concentrations and pore configurations.

(Oak Ridge National Laboratory, G. D. Wignall, H. R. Child)

19. Long Term Stability of Nuclear Fuels

Long-term stability of reactor fuel elements is important for safety and economics in the nuclear industry. One of the most important stability factors for UO_2, the most widely used fuel, is slow buildup of oxygen gas during power generation. Oxygen pressure and how quickly oxygen can migrate to the cladding (diffusion) determine fuel element stability. An ingenious technique to measure the diffusion coefficient of oxygen in UO_2 was devised. It is based on measurement of oxygen isotope ratios in isotopically enriched wafers of UO_2 that are separated by a thin membrane of molten uranium. Results from this experiment indicate that the diffusivity of oxygen in UO_2 is 100 to 1000 times less than had been estimated from previous experiments. This experiment establishes more reliable values for the thermal properties governing the stability of UO_2 fuel elements.

(Lawrence Berkeley Laboratory, D. Olander)

20. Studies of Sulfate Pollutant related to Acid Rain Sources

In an extensive set of experiments to characterize aerosols, it was found that sulfates produced in burning fossil fuel were richer in oxygen-18 than were sulfates produced in the atmosphere. Oxygen isotope radio measurements were subsequently made to determine primary and secondary sulfates in airborne sulfate samples and in snow and rain, and have resulted in new estimates of their concentrations. Primary sulfates are defined as sulfates that are formed before emission into the atmosphere as from fossil plants; secondary sulfates are formed after emission of sulfur into the atmosphere. Primary sulfates collected in the Chicago area from snow and rain were found to have a higher concentration by 4-5 over that previously accepted. These new findings indicate that previous assumptions concerning acid rain sources need to be reexamined. Further, the new isotopic analysis method should prove invaluable in U.S. and international programs to characterize acid rain and its sources.

(Argonne National Laboratory, B. Holt, R. Kumar, P. Cunningham)

21. Electromagnetic Measurements Track In Situ Oil Shale Retorting

Measurement of the electrical conductivity of oil shale in small scale laboratory experiments has led to a new phenomenological model that predicts conductivity changes during underground retorting of oil shale. The model was developed with the idea of obtaining remote underground images from high frequency electromagnetic measurements.

With the help of this new development, field experiments in an underground oil shale retort were designed and conducted. In this field experiment, sponsored by Fossil Energy, the new electromagnetic measurements were compared with measurements obtained with a more expensive and cumbersome method involving an array of thermocouples placed in the retort. The results indicate the electromagnetic method is not only cheaper but also more reliable. It is now possible to remotely pinpoint the location of an underground oil shale retort and simultaneously determine the temperatures in the retort zone.

(Lawrence Livermore National Laboratory, A. Duba, W. Daily, R. Lytle A. Piwinskii)

22. Vibrational Control for Increasing Productivity of Chemical Reactors

Controlled oscillation of the flow of chemicals into many chemical reactors can give as much as a five-fold increase in production rate over the rate practical without the oscillations. This new insight came from applying the concepts of vibrational control to continuous stirred tank chemical reactors, widely used to carry out heat producing reactions such as ammonia synthesis. Vibrational control is fundamentally different from feedback control; a simple physical example is stabilization of a rigid pendulum in a normally unstable upright position by oscillation of its point of suspension. Lasers and particle accelerators are currently often operated with vibrational control. The processes run in continuous stirred tank chemical reactors frequently suffer from product decomposition (or recombination) at normal operating temperatures. These problems can be minimized, according to the new theoretical developments, by oscillations which allow stable operation at lower than usual temperatures and higher than usual flow rates. Experiments are underway to demonstrate the method and explore its range of potential applications.

(Illinois Institute of Technology, S. Meerkov)

23. Production of Oxygen Enriched Air Using Liquid Membranes

A significant new development uses a liquid membrane to provide oxygen enriched air (80% O_2) in a single step. It is several times superior to any other membrane process. In this new approach, a liquid carrier binds oxygen on one side of the membrane and releases it on the other, in a way that is similar to hemoglobin. There are indications that this purification system has excellent stability and that recycling of the enriched product will result in nearly pure oxygen. Combustion accounts for over 90% of the U.S. energy consumption. The presence of nitrogen in combustion air (80% N_2) gives rise to a substantial energy loss in heating nitrogen and to air pollution by oxidation of nitrogen at high temperature. Both adverse effects can be reduced by enriching the air needed for combustion with oxygen. Many industrial processes also require nearly pure oxygen which is obtained by fractional distillation of air. The new process could lead to a more economic alternative. This research, is being transferred to the Division of Coal Gasification, Office of Coal Processing for further development.

(Bend Research, Inc., H. Lonsdale)

24. Use of Microorganisms to Remove Sulfur and Nitrogen from Fossil Fuels

The number of petroleum sources containing levels of nitrogen and sulfur contaminants low enough so that combustion of this fuel does not lead to significant environmental pollution is rapidly decreasing. Stocks of more heavily contaminated petroleum are in good supply and could satisfy a considerable portion of our energy needs if inexpensive and efficient methods for the removal of these contaminants were available. One approach to this problem is through biological purification of petroleum. More than ten isolates of bacteria which attack a number of organic nitrogen- or sulfur-containing compounds found in petroleum or synfuels have been obtained from soils and other sources. The bacteria were found to be capable of converting up to 98% of some of the contaminants to water-soluble products within 2-3 days. In the water-soluble form the contaminants can be removed readily. The bacteria carry out the oxidation of these compounds with a high degree of selectivity leaving the useful hydrocarbons unaltered. The bacterial genetic elements controlling these capabilities have been found to reside on plasmids, suggesting very favorable potential for applying genetic engineering techniques leading to a new biotechnology for decontaminating petroleum.

(University of Georgia, W. R. Finnerty)

25. Hydrogen Fluoride Used to Convert Cellulose to Sugar

A simple economic method of "cracking" cellulose to yield feedstock sugars remains elusive. In exploring a novel cellulose "cracking" method that uses gaseous or liquid anhydrous hydrogen fluoride, several clear advantages over conventional acid hydrolysis techniques were discovered. The hydrogen fluoride technique gave higher sugar yield than other acid hydrolysis procedures. It is a process that is faster, more simple and consumes less energy. Furthermore, it appears that most of the hydrogen fluoride can be recycled. These encouraging experiments carried out on a bench top scale need further optimization before scale-up can be contemplated.

(Michigan State University, D. Lamport)

26. Key Developments in Plant Molecular Biology

Two recent advances involving studies on the structure and function of plant genes requisite to the development of the "genetic engineering" of plants have been made. The studies are being done on maize which is one of the most important model systems for plant molecular biology. The rapid sequence determination of the nucleotide base "building blocks" in maize genes has been accomplished by the application of methods modified from those used in microbial systems. The second advance concerns the biochemical localization of a "control element" gene as a prelude to cloning it. Control elements are of great significance because they act to turn on and turn off, in a highly precise way, other genes which govern a variety of biochemical functions. Control elements are believed to act by the insertion of specific DNA sequences into particular regions of the chromosome. These advances should lead to the further development of methods to convey specific desired genes from one plant to another as well as the capability of bringing about specific alterations in plant genes as might be desired in the development of biomass producing plants.

(Brookhaven National Laboratory, B. Burr, F. Burr; University of Minnesota, J. Messing)

27. Coated Semiconductor Electrode Improves Possibility of Electrochemical Solar Cell

A new technique has been developed for electrodepositing a polymer film of polypyrrole on a polycrystalline n-type silicon semiconductor electrode. The treated electrode was used as the anode (positive electrode) in a cell containing a water solution of iron salts and an ordinary metal cathode (negative electrode). Upon illumination with visible light the iron was oxidized at the anode and reduced at the cathode, so that with no net change in the solution, electricity flowed in an external circuit. Untreated electrodes corrode sufficiently in a few seconds of operation to stop the flow of electricity. Initial tests of these coated electrodes were run for 120 hours with little change in their performance. Tests of power conversion indicated a 3% conversion efficiency, about one third that of a solid state device employing polycrystalline silicon. The important characteristics of this coating are its complete coverage of the electrode (providing the protection) and its high electrical conductivity (providing a path for the flow of electricity). Current research is exploring the properties of the polypyrrole film, its use to protect other semiconductor electrodes and its use in fuel-forming photoelectrochemical cells.

(Solar Energy Research Institute, A. J. Nozik, A. J. Frank, R. Noufi)

28. Breakthrough Experiment Measures Electron-Electron Interactions

Laser beam probing of energetic negative hydrogen ions (H^-) has led to the first precise measurements of the interaction between two electrons in the isolated ion. The experiments used the LAMPF ion beam to provide H^-, a species not commonly accessible by conventional laboratory methods, and a laser. The angle between the ion beam and the laser beam could be accurately controlled, so that the frequency (energy) of the photons in the moving reference frame of the ions could be varied. This phenomenon, called the Doppler effect, is commonly experienced when a stationary listener hears the frequency of a siren change as the siren approaches and then recedes from the listener. In the experiment, the energy range in which strong photon absorption (resulting in electron emission) took place was larger than that predicted by theory. This suggests that some physics was omitted from the mathematical formulation describing the H^- system. The new experimental results will aid in understanding the role of electron correlation (how electrons affect each other) in H^- and should stimulate new ideas toward better understanding of more complex ions. Examples are the highly ionized heavy atoms that contaminate fusion plasmas. Also, the negative hydrogen ion is of great practical interest because it is a desirable precursor to formation of neutral hydrogen beams that provide auxiliary heating of fusion plasmas.

(University of New Mexico, H. Bryant)

29. Two Discoveries Strengthen Scientific Basis for Catalyst Design

A better understanding of the detailed bonding interaction between the transition metals which are used as catalysts and substrates for synthesis gas ($CO + H_2$) conversions has resulted from two recent scientific discoveries. In the first, convincing evidence has been obtained favoring one of three proposed mechanisms for hydrocarbon chain growth in Fischer-Tropsch synthesis. The results clearly indicate that the chain growth occurs by insertion of CH_2 species into a metal alkyl bond. This insight is an important contribution to the design of catalysts of high specificity for conversion of synthesis gas into longer chain hydrocarbons. In the second, recent work has resulted in a kinetic method for obtaining values of metal-carbon bond strengths. These are very important in catalytic reactions involving the formation or isomerization of hydrocarbons. It has recently been shown that a kinetic method can be used to obtain values for chromium-carbon bond energies. Values for the energies of bonds between chromium and hydroxyalkyl groups have been obtained by measuring both forward and reverse rates of α-hydroxyalkyl metal-carbon bond reactions. These particular bond energies are especially important since hydroxyalkyls are believed to be intermediates in catalyzed H_2 + CO reactions which lead to hydrocarbon and oxygenated hydrocarbon products (Fischer-Tropsch synthesis).

(University of Texas, R. Pettit; Ames Laboratory, J. H. Espenson)

30. Mathematical Models of Turbulence

Turbulence in fluid flow is a complex and poorly understood phenomenon; but it is crucial in determining efficiency in combustion processes. This year a major breakthrough was made in solving the nonlinear differential equations that describe turbulence. New numerical methods were applied for the first time to provide accurate solutions to classes of energy related problems that were previously intractable using standard methods. Researchers supported by Applied Mathematical Sciences successfully modeled the combustion of gases in a cylinder and compared the numerical results with photographs obtained in laboratory experiments. The turbulent behavior of the combusting mixture is duplicated by the mathematical model, providing direct evidence that the model is accurate and that the numerical techniques are stable. These techniques can now be applied to more realistic geometrical configurations, such as engines, to provide more efficient and pollution-free designs.

Recently, mathematically similar techniques were applied to the "fingering" phenomenon that occurs when water or steam is injected into an oil reservoir for tertiary recovery. Fluid instabilities develop that cause the injected fluid to break through the oil too soon, limiting the amount of oil that can be recovered.

Unforseen but valuable spinoffs in apparently unrelated areas are common to mathematical research. This was amply demonstrated by the application of the turbulence modeling methods to explain how valves in the human heart are closed as a result of vortices in the turbulent flow of blood, when it appears that the valves are too weak to close with their own muscle power.

(Lawrence Berkeley Laboratory, A. Chorin; Courant Institute of NyU, J. Glimm)

Appendix E

MULTIPROGRAM NATIONAL LABORATORY ACCOMPLISHMENTS

March 10, 1982

AMES LABORATORY

- The Ames Laboratory developed efficient reduction and purification processes for uranium, thorium, the rare earths, zirconium, hafnium, yttrium, and vanadium. All of the processes have been adopted by industry, and all are in use today. Essentially all of the uranium used in the Western world has been prepared by the Ames process, and the entire rare earth industry is largely dependent upon the basic separations and chemical, metallurgical, and materials characterization achievements of this Laboratory (1940 to present).

- The development of the inductively coupled plasma atomic-emission spectroscopy method for multi-element analysis was carried out at the Laboratory. The method is very fast, requires minute amounts of sample, and permits simultaneous identification of up to 50 elements; for most of these elements, this method is more sensitive than any other. Commercial instruments based on this development have been introduced: six U.S. and eleven foreign companies are now marketing such instruments at a sales rate of about $100 million per year (1970s).

- Development of a ductile, composite superconducting wire suitable for large-scale magnets in the 12- to 14-tesla range was carried out by an interdisciplinary team of metallurgists and solid state physicists at Ames Laboratory. The material is easy to fabricate and has the high strength and strain tolerance needed for toroidal field magnets in Tokamak fusion reactors (1970s to present).

- The Ames Laboratory developed the basic science for sampling, isolating, and quantitating the trace organic compounds in water. The isolation techniques have increased detection power approximately 10,000-fold for most compounds of environmental interest. The methodology has been adopted nationally and internationally by government, university, and industrial laboratories (mid to late 1970s).

- Recently a reactive radio frequency sputtering method for the preparation of hydrogenated amorphous silicon films for solar cells was developed here. The method permits the preparation of large-area films needed for solar panels while retaining the careful control of the local environment of the hydrogen ions, which is needed for high performance.

- Very recently a method based on high-resolution solid state nuclear magnetic resonance in coal samples has been developed for determining the sizes of the polynuclear aromatic rings in the molecular structure of coal. These results, compared with similar results on liquid fuels produced from coal, are used to study the effects of the chemical processing steps in liquefaction (1978–1980).

ARGONNE NATIONAL LABORATORY

- Water-cooled nuclear reactor research, design, and development at Argonne National Laboratory contributed significantly to the establishment of the nuclear power industry and in the nuclear-powered submarine. The Laboratory still provides reactor and reactor waste safety information (1946 to present). This capability was applied to the following projects:

    1. design of the first land-based prototype submarine reactor,
    2. design of the first reactor using heavy water as a moderator and coolant,
    3. basic design of the Savannah River production reactors, and
    4. development of the boiling water reactor concept [Boiling Reactor Experiments (BORAX), Experimental Boiling Water Reactor (EBWR)].

- Liquid-Metal Cooled Fast Breeder Reactor (LMFBR) research, design, and development at Argonne provided the technology foundation for these reactors and continues to provide component and materials testing and evaluation. It has accumulated 16 years of LMFBR operational experience in the production of electricity. This research produced the following advances:

    1. design of the first successful breeder reactor (EBR-I), which produced the first usable amounts of nuclear-generated electricity;
    2. development of fast reactor and high-temperature reactor fuel materials; and
    3. development of the world's first transient reactor test facility (TREAT) to study fuel behavior during sudden power surges (1946 to present).

- A prototype superconducting linear heavy-ion accelerator is operational. When a total of seven modules are completed, the Argonne Tandem-Linac Accelerator System (ATLAS) will be able to provide 1.5-GeV particles, previously unavailable, that will improve understanding of nuclear binding forces (1979 to present).

- Intense Pulsed Neutron Source-I (IPNS-I) provides the world's most powerful source of non-reactor neutrons, which will be used to study radiation effects in fission and fusion reactor materials. Other applications will include areas of physics, chemistry, and biology (1971 to present).

- Zero Gradient Synchrotron (ZGS) acceleration of polarized protons was used to study spin-spin interaction between protons at high energy. Contrary to the existing belief, spin effects were shown to be large (1971–1979).

BROOKHAVEN NATIONAL LABORATORY

- The large particle accelerators that Brookhaven National Laboratory (BNL) has designed, built, and operated as national facilities have been the sources of many discoveries in particle physics which have led to a deeper understanding about the nature of matter. The first observation of a charmed baryon was made at BNL; and two recent Nobel prizes in physics, 1976 and 1980, were awarded for work carried out at BNL: the discovery of the J/psi particle in 1974 and the experiment which showed the violation of a fundamental symmetry principle in 1963.

- By the middle of the 1970s, sufficient data were obtained from a 600-ton solar neutrino detector situated 1 mile underground to show that either our current views of the details of the nuclear reactions generating the sun's energy are incorrect or that our understanding of the fundamental properties of neutrinos is not complete. Since both of these possibilities are of great interest, a new experiment designed to eliminate one of them is under way.

- The animal model developed at BNL, a specific species of rat, the Dahl S&R, was first used to show the genetic linkage between sensitivity to environmental stress, including dietary salt, and the likelihood of developing hypertension. These rats continue to be widely used for much of the present laboratory work on this disease.

- The invention at BNL of a procedure by which the short-lived radiopharmaceuticals such as ^{99m}Te and ^{201}Tl could be effectively distributed and used by the medical community started a new generation of nuclear medicine applications. These two isotopes account for approximately 75% of the domestic radiopharmaceutical business in the United States, a sales level of $85 million.

- The pioneering work on the therapeutic use of L-Dopa for the treatment of Parkinson's disease was carried out at BNL. This drug continues to form the foundation for the treatment of this disease today (early 1970s).

- The labeling of 2-fluoro-2-deoxy-*d*-glucose with radioactive ^{18}F at BNL and use of this radiopharmaceutical in conjunction with positron-emission transaxial tomography (PETT) has initiated widespread activity in many new areas of medical research. Regional metabolic activity at accurately determined locations inside the brain can now be measured. The technique has led to a much more detailed understanding of a whole range of phenomena (e.g., drug response) and diseases (e.g., senility, stroke, and schizophrenia) that affect the brain. The National Institutes of Health (NIH) are now supporting about ten centers to carry out this type of work (1976).

LAWRENCE BERKELEY LABORATORY

- The Lawrence Berkeley Laboratory (LBL) has been responsible for numerous major advances including the invention of the cyclotron, the linear accelerator, the synchrotron, and continuing contributions to new particle accelerator concepts and construction projects (1929 to present).

- The creation and identification of 15 new chemical elements, including plutonium, by nuclear synthesis was carried out by scientists at LBL (1940–1976).

- Particle research conducted by scientists at the Laboratory led to the discovery of the antiproton and numerous excited states of the fundamental particles (1955–1965).

- The Laboratory became one of the world's major centers of heavy-ion nuclear physics research by (1) adapting the 88-Inch Cyclotron to the acceleration of heavy ions (1971); (2) connecting the SuperHILAC heavy-ion accelerator to the Bevatron to make the Bevalac (1972); and (3) improving the Bevalac (1981) to provide acceleration of ions as heavy as uranium to multi-billion-volt energies, a capability unavailable anywhere else in the world. SuperHILAC, Bevalac, and 88-Inch Cyclotron accelerators serve as national facilities for nuclear physics and biomedical research (1971 to present).

- The LBL was responsible for the founding of the National Center for Electron Microscopy equipped with instruments of highest energy and highest resolution (1980 to present).

- The Laboratory was also responsible for the founding of the science of nuclear medicine (1935), the continued development of instruments and techniques for the beneficial use of gamma and particle radiations (1935 to present), and the exploration of use of heavy ions for treatment of cancer.

- The Laboratory has contributed significantly to discoveries and developments in high energy physics: for example, discovery of the ψ family of particles, the discovery of charmed particles, the design and construction (with Stanford Linear Accelerator Center) of the Positron-Electron Project accelerator, the design and construction of the Mark I and II massive detector systems, the design of the Time Projection Chamber superconducting magnet, and the development of stochastic beam cooling (1974 to present).

LAWRENCE LIVERMORE NATIONAL LABORATORY

Weapons

- Since its establishment in 1952, LLNL, in conjunction with Los Alamos and Sandia, has continued to function as an integral scientific and technical element of the nation's nuclear weapons program including all facets of nuclear weapon technology and the supporting scientific and engineering disciplines. Particularly, significant achievements have been made in such areas as reduction in size and weight, and enhanced safety, flexibility, and military effectiveness of nuclear weapons. These advances in design have enabled the defense community to provide the nation with increasingly effective warhead capabilities for its nuclear weapons systems.

Nonweapons

- Under inertial confinement fusion, LLNL developed the Excimer Transfer Laser and the rare gas oxide lasers (1972–75). Other significant advances were the first laser induced thermonuclear reactions (1975) and 1 billion and 30 billion reactions in the Argus (1976) and Shiva (1978) fusion devices. Significant progress was made toward thermonuclear conditions of a commercial power reactor with the compression of fuel to densities 150 times that of liquid deuterium (1979–80). Also, a preliminary engineering design for a reactor chamber with a liquid lithium wall was prepared that will permit fusion reactor design to last the life of a power plant.

- Within the Atomic Vapor Laser Isotope Separation (AVLIS) Program, researchers separated uranium isotopes (1974); demonstrated macroscopic uranium enrichment utilizing critical subsystems scalable to production plant size (1978); developed a high-power tunable (isotopically selective) laser operation (1981); and activated a full-scale uranium vaporizer unit (1981).

- Livermore's involvement in magnetic fusion research dates from the founding of the Laboratory in 1952. As lead laboratory for the National Magnetic Mirror Program LLNL achieved thermonuclear plasma temperature with near-classical confinement in the 2X-IIB experiment (1978); demonstrated the adaptation of the mirror concept to an efficient reactor design in TMX (1980); developed, with LBL large neutral beam systems used for heating plasma (1977); and developed large, high-field superconducting magnets Baseball II and Mirror Fusion Test Facility, MFTF (1981), which enhance related energy technologies like magnetohydrodynamics.

LOS ALAMOS NATIONAL LABORATORY

Weapons

- Established in 1943, Los Alamos National Laboratory (LANL) developed the first fission and thermonuclear weapons. In conjunction with Sandia and LLNL, LANL has continued to maintain U.S. superiority in all facets of nuclear weapons technology and supporting scientific and engineering disciplines. Enhanced safety, flexibility, and military effectiveness have been produced through a reduction in size and weight of the weapons. These advances in design have enabled LANL to provide increasingly effective warhead capabilities for integration into a number of defense systems serving every branch of service.

Nonweapons

- Examples of major Los Alamos accomplishments before 1970 include designing, building, and operating the world's first plutonium-fueled fast reactor and the world's highest temperature and power density fission reactors, thereby establishing possibilities for advanced fission systems and eventual process heat applications. Los Alamos also achieved the first laboratory demonstration of controlled thermonuclear fusion, thereby establishing the possiblity of eventual electricity production from fusion reactions.

- The Molecular Laser Isotope Separation (MLIS) Process for the enrichment of uranium has been developed to the point of demonstrating process feasibility. If developed to production scale, the MLIS process would result in a significant reduction in energy consumption and cost.

- Fast reactor fuels of plutonium carbide developed by Los Alamos successfully attained specific power production ("burnup") of over 150,000 mwd/ton (1981). This is much higher than that offered by present oxide fuels now used in breeder reactors. The new fuel has also demonstrated the capability of undergoing severe heating transients without performance degradation. The combination of the improved thermal, mechanical, and neutronic performance of carbide fuel could lead to significant savings in fast-reactor fuel fabrication costs and in overall plant and operating costs as well.

- Special plutonium fuels using a Los Alamos oxide of ^{238}Pu and ^{16}O now provide long-life, stable, low background heat sources which generate electricity for experiments on the moon and on the Voyager spacecraft. Newly developed general purpose heat sources employing the same material will be combined in modular arrangements to power the Galileo Deep Space Probe and the Polar Orbiter solar studies mission. The same material, used in smaller radioactive heating units, has numerous applications.

- Heat pipes are simple devices, largely invented and perfected at Los Alamos, which make possible very high heat transfer rates over very small areas. Performance and light weight led to their early use for temperature equilibration in satellites and spacecraft. Heat pipes solved a critical problem on the Alaska pipeline, where their use at every pipe support prevents the pipeline from sinking into the permafrost. They provide efficient heat recovery in industries and allow safely separated inlet-outlet airflows while recovering heat at hospitals. New applications emerge continually. Recent Los Alamos work has extended heat pipe capabilities to very high temperatures (1500 K) for potential uses ranging from industry to heat radiators for nuclear electric space power.

OAK RIDGE NATIONAL LABORATORY

- Oak Ridge National Laboratory (ORNL) served for over 30 years as the principal developer and reference source for models and techniques to estimate radiation doses received by humans. Essentially all nations have uniformly adopted usage of the ORNL models and techniques through the recommendation of the International Commission on Radiological Protection (1940s to present).

- The Laboratory has developed advanced centrifuge techniques for producing pure vaccines and for performing rapid medical diagnoses. These are now in wide-scale commercial use (1965–1975).

- The development of radionuclide production for nuclear medicine applications was initiated at ORNL, and, in conjunction with medical schools and hospitals, the Laboratory developed efficient radiopharmaceuticals as imaging agents to study heart disease and locate brain tumors (1945 to present).

- The first heavy-ion cyclotron was constructed at ORNL, and the field of heavy-ion physics was founded by establishing the general properties of heavy-ion elastic scattering, transfer reactions, and compound nuclear reactions (1950 to present).

- Crucial determinations were made of neutron radiation damage, including radiation-induced creep, in metals and alloys; contributions in this area have been necessary for the development of nuclear reactors (1949 to present).

- Theory and supporting data for the design of heavy section steel vessels were developed at ORNL. The results of this program have provided an assurance of safety necessary for the light-water reactor (LWR) pressure vessel, which has been accepted by regulatory bodies both in the United States and other countries (mid-1960s to present).

- The Laboratory provided rapid and extensive assistance during the Three Mile Island incident, from the beginning until now. Radiochemical, chemical, and isotopic measurements were made, along with a variety of physical tests. ORNL developed the process flowsheet for the cleanup of the water from the containment building. ORNL also resolved the question of why iodine releases were so low and showed that much lower iodine releases than previously predicted would occur in many LWR accident scenarios (1980 to present).

- For nuclear fuel reprocessing, ORNL developed Purex (1953), Thorex (1958), and Remotex (1980). Purex and Thorex processes are now used in all known fuel reprocessing plants throughout the world. Remotex is a fully remote processing concept which has been used for most radioisotope systems and also has been applied to the handling of hazardous materials such as carcinogenic compounds.

PACIFIC NORTHWEST LABORATORY

- The Pacific Northwest Laboratory (PNL) successfully demonstrated the immobilization of high-level waste from the nuclear fuel reprocessing of six commercial fuel assemblies in a stable glass form for storage. The process is being transferred to the Savannah River Laboratory for use in the Defense Waste Processing Facility (1976–1979).

- For over 30 years the Laboratory has conducted experimental research that has led to major improvements in nuclear fuel performance, plant safety, and system reliability. This research has included a cooperative program (1973–1975) with Japan and several European countries that led to resolution of fuel densification questions threatening shutdown of numerous nuclear power plants in the United States and throughout the world.

- The Laboratory established the technical and environmental basis for the private-sector use of plutonium and uranium oxide fuels in light water reactors (1960–1970). The technology has been adopted by one corporation as a new venture that has grown to a multihundred million dollar fuel reload business with a billion dollar backlog (1967–1975).

- Electropolishing and vibratory-finishing techniques for decontaminating metal surfaces were developed at PNL. These techniques are being used for the cleanup at Three Mile Island; they have been incorporated in mobile decontamination units operated by seven commercial companies; and they are factored into decontamination plans of most DOE sites (1975–1980).

- An advanced cooling-tower process that uses little or no water was developed; this is an important alternative for arid western states or other regions of uncertain future water supply. The concept is being demonstrated by the private sector at a utility power station and holds the potential of 30 to 40% cost reductions over existing dry-cooling technology (1974–1981).

- High-rate and large-volume sputtering processes have been developed for the versatile fabrication of special-purpose materials and coatings. The technique has been used for coating turbine blades for increased reliability, fabricating materials for high-energy-laser mirrors, and trapping krypton gas in metals in order to meet release criteria for nuclear reactors and other nuclear facilities (1969 to present).

SANDIA NATIONAL LABORATORIES

Weapons

- Since its establishment in 1949, Sandia has developed safe, reliable, deliverable, field-ready weapons using the nuclear devices developed by LANL and LLNL. Sandia's weapons research and development includes arming, fuzing, and firing systems; command and control systems; and the structural and aerodynamic designs. Significant advances in safety, security, and flexibility of those systems as well as in miniaturization of components and protection against hostile environments have been made. Sandia has also been instrumental in extending component shelf life, thus greatly reducing stockpile maintenance costs. The Laboratory performs these functions for all nuclear weapons in the stockpile. About 75% of Sandia's staff is engaged in defense activities.

Nonweapons

- In a program initiated in the early 1970s, Sandia has discovered a family of transparent electroptic ferroelectric ceramics based on lead lanthanum zirconate titanate (PLZT) and has developed unique solid-state devices based on these materials. The applications include image storage, processing, and display devices; light valves and shutters (e.g., flashblinders and welding goggles, spectral and variable density filters); and numeric displays. Over 20 companies and laboratories in the United States and abroad now have active research and development programs on PLZT materials and devices.

- After conducting systems studies of fossil and geothermal processes, Sandia developed more than 12 devices and processes now widely used by industry. Examples are high-temperature microcircuits, coring devices, new drilling muds, new hardrock drill bits, and a downhole combustion device for injecting steam into oil-bearing formations. Since about 80% of this country's heavy oil deposits will be recovered using thermal energy, it is significant that downhole steam generators use less fuel, create less pollution, and recover more oil from greater depths than surface generators. Several commercial firms are in design and manufacture of the device (1974–1982).

- Sandia has managed a significant fraction of the national solar energy program. The Laboratory's systems studies and experience with costs of hardware construction and operation revealed market limitations that were not commonly recognized nor publicized. Over 20,000 industrial and political decision makers have been extensively briefed on the results of this work (1972 to present).