SOME EXAMPLES OF ACCOMPLISHMENTS

UNDER THE BASIC ENERGY SCIENCES

PROGRAM DURING 1984

FEBRUARY 1, 1985

Some Examples of Accomplishments Under the Basic Energy Sciences Program during 1984

February 1, 1985

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

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1. Metallic Glasses Now Synthesized Without Ultrarapid Quenching

Metallic glasses differ in structure and properties from metals. Metals normally have a crystalline structure with atoms in periodic arrays called lattices. In contrast, atoms in glassy metals do not form periodic arrays; their distribution is random. Originally devised a quarter of a century ago, the technique to produce amorphous or glassy metals required cooling the molten metal about one hundred thousand times faster than had previously been possible. Rapid cooling was the only way to prevent mobile atoms in the molten metal from rearranging themselves into crystal lattices. Recently it has been discovered that metallic glasses can be synthesized at low temperatures without quenching by directly introducing certain rapidly diffusing species into crystalline materials. Systems studied so far include hydrogen diffusion in some intermetallic compounds, gold diffusion in lanthanum, nickel diffusion in zirconium metal, and others. The common process in all of these systems is that one of the elements, viz., hydrogen, gold, and nickel in the above examples, diffuses very rapidly in the other at low temperatures. The rapidly diffusing species induces a phase instability which, because of the low temperatures, results in an amorphous structure rather than a crystalline structure.

Since metallic glasses have normally been produced by rapidly quenching liquid streams, metallic glasses actually have been limited in physical shape to very thin films or ribbons. Thus, despite their enhanced physical and mechanical properties over normal crystalline materials, applications of glassy metals have been limited to only those where such films or ribbons can be used. This new discovery thus has at least two significant implications.

First, from a scientific point of view, the discovery that equilibrium crystalline materials can be induced to transform to nonequilibrium amorphous materials is an exciting development. Second, it portends the possibility of preparing bulk (as opposed to thin ribbon) metallic glasses, thereby making metallic glasses with their enhanced magnetic and other properties accessible for a wider range of applications.

(California Institute of Technology, W. L. Johnson)

2. Stress Corrosion Cracking in Ductile Metals Explained By Localized Brittle Cracking and Altered Surface Layers

It has been experimentally observed that stress corrosion cracking (SCC) proceeds up to one thousand times more rapidly in ductile metal alloys than predicted using current theories. The discrepancy has been explained on the basis of localized brittle cracking which does not involve hydrogen, but which involves altered surface layers. This new mechanism was found in experiments on stress corrosion cracking of brass; the experiments coupled novel electrochemical and mechanical testing and nondestructive evaluation techniques and demonstrated that each increment of crack growth is accompanied by acoustic emission and a series of current transients. Molecular dynamics modelling, using two dimensional computer simulations of a crack in brass under conditions corresponding to those determined experimentally, corroborated the localized brittle cracking explanation.

This definitive delineation of a new brittle cracking mechanism in stress corrosion cracking both demonstrates that altered surface layers can change the fracture mode from ductile to brittle in normally ductile metals and resolves heretofore controversial experimental results obtained for some ductile metals.

(Brookhaven National Laboratory, K. Sieradzki, R. C. Newman, and H. S. Isaacs)

3. Ductility of New High Temperature Alloys Improved by Controlling Grain Boundary Chemistry

Nickel aluminide is an intermetallic compound that, until now, has been considered intrinsically brittle. Ductility levels useful for structural applications of nickel aluminide, however, have been observed and their occurrence has been definitively related for the first time to segregation of boron at boundaries between adjacent crystals in polycrystalline aggregates. The grain boundary concentrations of boron, aluminum, and sulfur in nickel aluminide have been measured using state of the art surface analytical spectroscopy techniques. The microchemistry data have been correlated with the macroscopic ductility of the material and the results are clear. Tensile ductility increases with increasing boron levels and decreasing sulfur and aluminum levels. Of particular importance, grain boundary segregation of boron is favored over sulfur when both are present in the alloy, so that conventional processing of materials in which minute levels of sulfur remain can be used.

This scientific result has major implications for alloy design. A new high-temperature oxidation resistant material, better than present superalloys, has been developed which can be produced by conventional casting and forming methods of alloys with modestly tightened composition limits. In the long term, understanding grain boundary microchemistry and relating it to the ability of grain boundaries to accommodate deformation without fracture underpins the development of all alloys. Brittle intergranular failure is the most significant failure mode for alloys in very long-term high-temperature service.

The potential of this aluminide has already been recognized by an IR-100 award as well as industrial interest in producing this material.

(Oak Ridge National Laboratory, C. T. Liu and C. L. White)

4. Advanced Electron Microscope Machines Holes and Slots in Thin Films to Atomic Dimensions

A novel machining method exploiting directed electron beam processing has been developed for boring holes and cutting slots in thin films with dimensions corresponding to those of ten atoms. This unique development permits machining to a dimension one thousandfold smaller than obtainable with commercial practice. This accomplishment was achieved by the use of a special electron source in a state-of-the-art electron microscope which focusses a very small, extremely high power electron beam on materials. Normally, the power level is low so that the material can be examined in the microscope. Above a threshold level, however, machining occurs in some materials, in particular, the aluminum oxides studied in this work.

This accomplishment has both scientific and technological importance. The fundamental behavior of atomic-dimension structures can be studied in a regime not heretofore accessible, namely, where the dimension of the specimen is smaller than critical distances controlling properties in bulk specimens. Wholly new technological vistas are opened up by this result--but new manufacturing concepts rather than refinement of current ones will be needed to exploit it. One potential application is the development of computer memories with storage densities one millionfold greater than presently possible, which will permit an enormous increase in complexity of problems to be studied. This new capability is possible only with advanced electron microscopes, and a patent application has been filed.

(University of Illinois, M. E. Mochel, J. A. Eades, C. J. Humphreys, M. Metzger, J. I. Meyer, J. M. Mochel)

5. Nuclear Magnetic Resonance Technique Broadened to Applications in Zero Magnetic Field

An important new use of nuclear magnetic resonance (NMR) as an instrument for science, technology, and medicine has been developed. NMR has been relatively weak in providing structural information on solids--e.g., how a material like a catalyst or a new alloy is constructed. With an amorphous substance like glass, or a polycrystalline one like zeolite catalysts, a broad, relatively featureless spectrum that contains little or no structural information is obtained because each "crystallite," or individual grain, of the substance has its own random orientation to the magnetic field. The new method developed, called "zero field NMR", cycles the sample between high magnetic fields and zero field. The extra resolution is achieved by measuring the spectra at zero field and allowing the nuclear spins themselves to act upon each other. With this resolution, the NMR spectrum of a powder becomes crystal-like, with clear, definite peaks, while amorphous materials have broad resonances characteristic of their short range order.

Zero field NMR promises to extend NMR to the analysis of such important industrial and biological materials as catalysts, plastics, and human tissue.

(Lawrence Berkeley Laboratory, A. Pines, D. Weitekamp and coworkers)

6. New Conceptual Basis Improves Prediction of Deformation Behavior of Metals

Combined theory and experimental measurements on large deformations (plasticity) of metals has led to a new "crystallographic" basis for deriving quantitative stress-strain relationships for polycrystalline metals. The conceptual difference between the old and new models for large strain plasticity of metals is significant--the new approach considers highly elongated grain shapes and favored orientations of planes in each grain with respect to local deformation, which is physically more realistic than earlier models which did not consider either grain shape or crystallographic orientations. Constitutive relations obtained with the crystallographic basis give substantially improved agreement between predictions of behavior and experimental results for brass and aluminum, particularly for loading conditions which are complex or involve changes from one stress state to another. In addition, the orientation of the crystal lattice in each grain of the aggregate was correctly predicted for the first time, confirming the physically realistic nature of the new model.

The validity and physical basis of the new model provide two improved capabilities heretofore governed by phenomenological models and empirical "rules." First is the ability to accurately extrapolate beyond an existing data base which must be obtained experimentally and, for complex conditions, at great expense. Second is the ability to use this extrapolation capability to predict failure criteria during metal working operations and thus avoid costly failures.

(Los Alamos National Laboratory, U. F. Kocks and M. G. Stout)

7. Advanced Neutron Scattering Techniques Developed for Studies at Very Low Temperature (.0027°K) and for Hydrocarbon Investigations

Both steady-state nuclear research reactors and spallation neutron sources are providing advanced capabilities in the effort to discover new properties of materials utilizing the unique capabilities of the neutron as a probe of matter. Using a steady-state reactor, nuclear ordering in praseodymium copper ($PrCu_2$) and holmium vanadate ($HoVO_4$) was observed for the first time at temperatures as low as 2.7 thousandths of a degree (.0027°K). These measurements were made possible by the use of a cryogenic dilution refrigerator together with a superconducting magnet which allowed these extremely low temperatures to be reached. At these temperatures, approaching absolute zero, fundamental properties of condensed matter, where atomic motion is nearly totally eliminated, can be obtained. This kind of information is important not only for the new properties discovered, but also for insights into the potential design of new materials with unusual properties. This experiment was part of a joint U.S.-Japan effort at Oak Ridge National Laboratory.

Utilizing the higher energy (epithermal) neutrons available from a spallation neutron source, new inelastic neutron scattering results were obtained from a series of hydrocarbons. Vibrational modes in this new high energy range were measured in butane and provided new structural information about that important hydrocarbon. The exploration of vibrational properties of hydrocarbons in this heretofore inaccessible energy range, gives new information that is important to advanced oil well logging diagnostics in the exploration of petroleum. In addition, the measurements provide new fundamental information about the hydrocarbons themselves. These experiments were part of a joint effort by Argonne National Laboratory and Schlumberger-Doll scientists.

(Oak Ridge National Laboratory, R. M. Moon and R. M. Nicklow; Argonne National Laboratory, D. L. Price; Schlumberger-Doll, W. Nelligan; Japan, S. Kawarazaki)

8. Ceramics Found to be Ductile Under Isothermal Forging Conditions

Two commercial glass ceramics have been found to be extremely ductile when mechanically tested at elevated temperatures under conditions that simulate isothermal forging. Each of these two materials contains a viscous glassy phase at grain boundaries at the testing temperatures of 1050° to 1150°C; the viscosity of the glassy phase is high in one and low in the other. The stress state, strain rate, and temperature were chosen so that fundamental information for an actual isothermal forging process could be obtained. The experimental results show that: (1) both materials are essentially infinitely ductile in uniaxial compression at ambient pressure, (2) the material containing the low viscosity glass phase can be deformed to nearly 400 percent elongation in uniaxial tension, and (3) with superimposed hydrostatic pressure the material containing the low viscosity glass can be essentially infinitely ductile even in tension.

This discovery suggests that under proper conditions, ceramics with select microstructural features may be sufficiently ductile to permit fabrication of components from them by isothermal forging. This is an important potential forming option since machining of ceramics is both very expensive and has a propensity to produce flaws that lead to unacceptable fracture. Hot-isotatic-pressing, which may be used for near-net-shape forming, has difficulties because large amounts of shrinkage occur during densification making it difficult to produce parts with close tolerances. Metallic superalloys which have been developed for high temperature applications are formed into shape by isothermal forging, but in order to apply the same technology to ceramics it is necessary that ceramics be ductile.

(Cornell University, R. Raj and J-G. Wang)

9. Theoretical Calculations Provide Important Thermodynamic Data for Atmospheric Chemistry Research

With recent advances in computers and theoretical methods the structure and stability of small molecules can be calculated to the best accuracy available from experiment. Such computations can provide thermodynamic data for molecules which are difficult or impossible to study experimentally. These calculations have great potential in the area of environmental chemistry where the thermodynamics of many postulated reactions, which have not been studied experimentally, are necessary to model atmospheric processes, such as acid rain formation. The energetics for the reaction of N_2 with an H atin to form N_2H has been calculated very accurately. The N_2H molecule is a postulated intermediate in acid rain formation as well as in other atmospheric and combustion processes; although, it has not been detected experimentally. A second problem which has been investigated is the energetics for the reaction of CO_2 with H_2O to form CO_2:H_2O. The CO_2:H_2O molecular complex is thought to be involved in the greenhouse effect occurring in the earth's atmosphere, but, again, little is known experimentally about its relative stability and spectroscopic properties.

The calculations on the N_2 + H "reaction surface" indicate that N_2H is probably not an important intermediate in atmospheric or combustion chemistry as had previously been postulated by other workers. The calculations on the CO_2 + H_2O "reaction surface" have provided thermodynamic data for the formation of the CO_2:H_2O complex which can be used as input for models being developed to evaluate the greenhouse effect. These data have also provided estimates of the vibrational frequencies of the complex to aid in its spectroscopic detection. These computations illustrate the potential usefulness for *ab initio* "reaction surfaces" in atmospheric chemistry.

(Argonne National Laboratory, L. A. Curtiss and D. L. Drapcho; Carnegie-Mellon University, J. A. Pople; Canisius College, D. Pochatki)

10. New Catalyst Simplifies Direct Conversion of Carbon Monoxide and Water to Methanol

Basic research on homogeneous catalysis, e.g., catalysis induced by catalysts dissolved in solvents, has led to the discovery of a new catalytic system that can promote the direct conversion of carbon monoxide (CO) and water (H_2O) to the fuel, methanol. This conversion can be made to proceed at temperatures and pressures much lower than heretofore necessary for converting CO to methanol. In fact, the yield of methanol is higher with this new catalyst at a pressure of only 10 atmospheres than it is at 100 atmospheres using the present commercial process. Equally or more important is the fact that the new catalytic sequence uses water instead of the far more expensive hydrogen presently required for methanol synthesis. This very promising discovery involves catalysts which are lead compounds dissolved in molten salts. The salts are formed by sodium or similar metals and formic acid. The formate salts and, of course, the lead catalyst are not consumed in the process.

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

11. Instrumentation Developed for Measurements Underlying Safety and Efficiency of Power Stations

A new method has been developed for in situ, noninstrusive, rapid and non-destructive measurement of the void (bubble) fraction in flowing liquid/bubble systems. It should be especially useful for distinguishing between fundamentally different types of boiling in nuclear and other power reactors, important information for maintaining efficient and safe operation. The concept is based on a sophisticated technique known as Fourier Transform Nuclear Magnetic Resonance, using a nonuniform magnetic field. It allows measuring bubble size, bubble growth (or shrinkage) and bubble velocity, with good dimensional resolultion and with rapid repetition, up to every 36 thousandths of a second. Void densities can be measured for both steady and unsteady flow, with resolution in both time and space. While the method is, so far, limited to one dimensional measurements, it is expected that it will be extended to three dimensions, which would provide widely applicable additional information: bubble shapes and merging or breakup of bubbles.

(University of North Carolina, R. E. Saxe)

12. Increasing the Temperature-Time Series Data Base

The data base for the Northern Hemisphere temperature-time series has been extended back to 1851. Previous data bases began in 1880 to 1900. Additional new records have been obtained worldwide from libraries, archives, and weather data centers. The number of sites for the period 1851 to 1900 was doubled over that of earlier data bases. The improvement in coverage during the late 19th century has resulted in a diminution of the apparent coolness of the period, particularly in the 1880s. The sparse geographic coverage in the original data set for this period resulted in temperature averages that were about 0.1°C lower than the revised values.

On the basis of the extended record, it appears that temperatures remained fairly constant during the second half of the 19th century at close to these levels that prevailed during the 1900s and 1910s, with no temporal fluctuations as have been observed during the 20th century. There is some evidence of a warm period during the first years that records were kept, but this may simply be a result of the restricted spatial coverage during that period. This matter is under investigation, because the occurrence of a period of warmth during the preindustrial period is significant for the detection of CO_2-induced warming.

Data from the 20th century data base are consistent with previous documentations, showing the approximate 0.5°C warming from 1910 to the mid-1940s followed by slight cooling through the early 1970s. A warming trend continued from the early 1970s to the present, with 1981 being the warmest year on record (since 1851) and 1983 being the fourth warmest.

(University of Massachusetts, R. Bradley; University of East Anglia (Norwich, United Kingdom), T. M. L. Wigley)

13. New, Surprising Insight into Combustion Chemistry

The first step in burning hydrocarbon fuels is often the chemical reaction which takes place between an oxygen molecule (two oxygen atoms bound together) and a molecule of the fuel which has lost a hydrogen atom, referred to by chemists as a hydrocarbon radical. But such reactions are hard to study, because the hydrocarbon radicals are hard to prepare in a manageable experimental environment. Recently, ethyl radicals (ethane minus a hydrogen atom) have been prepared with a laser-initiated photochemical method. Their reactions with oxygen molecules have been studied from room temperature up to nearly 1300° C. Experimental results did not support previous assumptions about the chemical mechanisms and rates of these reactions. The expected first step, oxidative breakup of the ethyl radical, does not take place. Instead, the oxygen molecule adds onto the radical, to form a peroxide. The rates of reaction actually decrease as the temperature is raised, so that, at combustion temperatures, the rates are considerably different from those assumed until now by modelers attempting to describe combustion processes. These new experimental results should contribute to improved models, leading to more effective use of present and future fuels.

(Illinois Institute of Technology, D. Gutman)

14. Solid State Electronic Devices for Use at Very High Temperatures

Most transitors in common use quit working when heated above about 200°C. However, progress is being made in building solid-state electronic devices tailored for use at high temperatures. Critical needs for these devices are well-known, for example in reliable instrumentation for jet engine control, geothermal well-logging, and controls for nuclear power plants.

In a major advance, a device called a semiconductor controlled rectifier--a switch--has functioned while red hot, that is at 550°C. This breaks the record for operating temperature for semiconductor devices. This controlled rectifier is a member of a family of devices formed from alloys of gallium, phosphorous, arsenic and aluminum now under intensive study for future energy related applications. Other family members, e.g., transitors and diodes, can also now be expected to function up to 550°C.

This research on instrumentation operable at high temperatures paves the way for widespread advances in measurement methods and process control in hostile environments.

(Sandia National Laboratories-Albuquerque, T. E. Zipperian)

15. Electrochemical Processes Identified as Mechanisms of Wear of Machinery

Until recently it was commonly thought that wear of bearings, gears and other moving machine parts is due mainly to mechanical and chemical causes. Much is known about wear due to abrasive particles, surface imperfections, and corrosion.

In a series of very careful experiments, it has been shown that wear due to electrochemical effects can be about the same as that due to purely mechanical causes. Thus it was found that tool marks or polishing scratches on metal surfaces in contact with one another and moving past each other in a lubricant give rise to localized electric currents much like tiny short-circuited batteries. The accompanying electrolysis wears out the surface at a high rate.

This new knowledge promises new approaches to reducing wear problems in machines. For instance some additives to the lubricant can reduce the electrochemical action and thus lessen damage to the metal surfaces. Results of this research will contribute to increased lifetime of machines used in energy production and utilization.

(Electrochemical Technology Corp., T. R. Beck)

16. Process Design and Control Strategies for Enhanced Energy Efficiency and Productivity Developed

In the past ten years fast changing economic conditions have forced engineers to design process plants which run efficiently not only under some nominal conditions, but also when varying inputs, e.g., price of energy, dictate changes in the way the plant is run.

Recent basic research on adaptive control systems has advanced to the point at which there is taking place a rapid transfer of knowhow from universities to industry. Notable innovations from this research include the first general method for rational synthesis of heat exchanger networks, which is important for better use of process heat in industry. Also, newly found theoretical methods for "resilience" assessment of heat distribution systems have been applied in realistic cases; "resilience" tests the reliability of control systems subject to uncontrollable disturbances. Further, stable use of non-linear controllers has been shown where linear control systems failed to stabilize the system operation.

The results of this pioneering work on process design and control will have a long-term impact on adaptive control research as well as on improving energy use by industry.

(University of Wisconsin, M. Morari, W. H. Ray and D. F. Rudd)

17. New Interpretation of the Volcanic Eruption Process

Combined geophysical techniques and drilling have resulted in several major discoveries this year in the Long Valley caldera region. The Inyo Domes form a line of volcanoes extending northward from the main caldera structure. These volcanoes are the youngest (600 years old) extrusion of the Long Valley magma system. Three DOE drilling projects have penetrated (1) a lava flow at Obsidian Dome volcano, (2) the magma conduit directly under Obsidian Dome, and (3) the deeper dike system that fed magma to the entire Inyo chain. Results to date include: a totally unexpected thermal anomaly persisting in the conduit since the 600 year old eruption; a first-ever direct observation of the 60m diameter conduit consisting of a 30m central channel through which lava flowed freely to the surface and an outer section of fragmented wall-rock intruded by magma; a new interpretation of the eruption process as an extrusion of outgassing silicate foam followed by a cooling period of bubble collapse and welding of glass fragments at the surface to form the currently homogeneous obsidian "lava flow". A full suite of cores and logs were taken in all three holes, and the two deeper holes were successfully cased for future geophysical experiments. Detailed analyses of core and geophysical data are currently under way, but it is already clear that the BES/Geosciences investigations are pioneering an unprecedented scientific understanding of the subsurface anatomy of magma-geothermal systems necessary for the efficient development of their vast energy resources.

(Sandia National Laboratory-Albuquerque, J. C. Eichelberger)

18. Geologic Evidence on the Conditions of Petroleum Formation

Rock samples obtained by drilling into the Green River Shale, an oil producing layer in the Uinta Basin of Utah, has provided direct geological verification of the rate and temperature conditions of petroleum formation. The shale contains kerogen (an organic precursor of petroleum) where it is exposed at the surface on the edge of the Uinta Basin. The same rock layer produces oil from depths of 12,000 to 16,000 feet inside the basin. By combining measurements of the state of compaction of shale samples recovered from drilling to successive depths with data on temperature as a function of depth, investigators were able to reconstruct the time vs. temperature history of the Green River Shale. For the oil producing zone, the average heating rate and maximum temperature achieved during the kerogen to petroleum transition were 5°C increase per million years and 155°C, respectively. This geological reconstruction of the natural conditions of petroleum formation is an excellent agreement with laboratory experiments on the chemical kinetics of converting kerogen to petroleum which indicate a very pronounced maximum in the rate of conversion in the range 150-160°C when the laboratory heating rates (necessarily much faster by many orders of magnitude) are extrapolated back to the natural rate. Because large extrapolations of laboratory data invariably introduce uncertainties about their applicability to natural phenomena, an independent geological confirmation is particularly significant in furthering our understanding of the origin of this fossil fuel.

(Lawrence Livermore National Laboratory, A. K. Burnham)

19. New Free-Electron Laser Amplifier Reaches High Power Levels

Microwave radiation power levels were boosted more than 250,000 percent in a free-electron laser amplifier. A microwave signal was sent through the unique laser amplifier raising the signal's power from 30,000 watts to more than 80 million watts. The amplified signal was measured by three different methods to be certain of its immense power output.

This is the first operation of a free-electron laser as a high-gain microwave amplifier. Previous experiments achieved similar high power microwaves, but they required an additional magnetic field that cannot be used for shorter wavelength radiation.

A free-electron laser amplifier is a device that can transfer energy from a beam of electrons travelling at near light speed (186,000 miles per second) to a beam of electromagnetic radiation, such as microwaves or visible light. The added energy increases the intensity of the electromagnetic beam.

The advantage of a free-electron laser is its efficiency in converting electrical energy into laser light and its ability to be tuned over a wide range of wavelengths. This research offers the additional benefit of being able to produce high-powered pulses of laser light.

Microwaves from a free-electron laser might drastically reduce the length and power requirements of linear accelerators, and could also help confine the fuel in certain types of magnetic fusion reactors.

Most significant to the researchers, however, is their expectation that the demonstration of their high-gain free-electron microwave amplifier will lead to success at shorter wavelengths along the electromagnetic spectrum, including infrared, visible and ultraviolet light, where the amplifier could be used for many laser applications.

(Lawrence Berkeley Laboratory, A. M. Sessler and D. Prosnitz)

20. Large Concentrations of Soot Found in Arctic Air

Large concentrations of soot have been measured at ground-level stations throughout the western Arctic; modeling studies indicated that the soot could lead to heating effects over polar ice. The soot may be responsible for the warming trend indicated by the Arctic temperature-time series which others have attributed to the carbon dioxide (CO_2) buildup.

One of the major uncertainties in modeling the effects of the Arctic haze on the solar radiation balance has been limited knowledge of the vertical distribution of graphitic carbon particles (soot) and their associated solar and infrared absorption coefficients. During 1983 and 1984, the first measurements of such distribution in the Arctic atmosphere were obtained. These measurements were achieved with a new instrument, called an aethalometer, designed at LBL that is capable of determining soot concentrations on a real-time basis.

Part of the data base obtained in 1983 has been analyzed, yielding the following results:

1. Substantial concentrations of soot were found throughout the Arctic atmosphere (i.e., in the Alaskan, Canadian, and Norwegian Arctic areas and the North Pole).

2. Vertical profiles of soot can show either a strongly layered structure or an almost uniform distribution to 8 kilometers (26,000 ft). Concentrations of particles within layers can be as large as those found at ground level in typical midlatitude urban areas.

3. A comparison of the vertical profiles with ground-level measurements indicates that peak concentrations aloft can be significantly greater.

4. The absorption optical depths associated with these vertical profiles are large enough to cause a substantial change in the solar radiation balance over a highly reflective surface such as polar ice.

5. Results of initial modeling studies with the new data have indicated that the soot could be one of the causes of the Arctic warming trends. (Lawrence Berkeley Laboratory, H. Rosen; Lawrence Livermore National Laboratory, M. C. MacCracken)

21. Carbon Dioxide Improves Water-Use Efficiency of Plants

Elevated levels of CO_2 cause increased plant photosynthesis. In addition, stomata (small pores in the leaf through which CO_2 and water vapor are exchanged) partially close in response to increased levels of CO_2, and this decreases plant water loss (transpiration). A concept now being confirmed by new data is that improved water-use efficiency* (WUE) because of elevated levels of CO_2 will measurably increase growth and dry weight gain of plants. This is especially important in situations of low-water availability.

New results of research on the response of plants to CO_2 provide improved quantitative values of photosynthetic WUE for several crops and native species. These results are based on research on whole plants that have been continuously exposed to elevated levels of CO_2 in containment situations that approximate normal field conditions (natural light and temperature). For soybeans and several other species grown inside such containment, it is clear that increased levels of CO_2 cause a doubling of the WUE, and for field-grown corn, the WUE may increase by 35 to 100%.

The accumulating experimental evidence of improved WUE is an important finding for agriculture and ecology because water stress is often regarded as the single most limiting factor for plant growth. Implications of improved WUE include the protection of plants from drought and other stresses, and

* The conventional expression of the efficiency of water to fix carbon is WUE = carbon fixed/water consumed

possibly reduction in the quantity of water required for the plant to complete its life cycle or to produce harvestable yield. Modified WUE could affect water requirements for irrigated croplands and may indirectly affect the distribution of natural plant communities. The possibility has also been proposed that CO_2 may function as a widespread antitranspirant, thereby making water available for other purposes.

(U. S. Dept. of Agriculture; Agronomy Physiology Lab-Gainesville, Florida, H. Allen; Air Pollution Effects Lab - N.C. State, H. Rogers; Crop Simulation Lab - Mississippi State, B. Acock. Lawrence Livermore National Laboratory, J. Shinn)

22. <u>New Theoretical Approach Advances Understanding of Combustion Chemistry</u>

Increased understanding of the combustion process is needed to improve the use of hydrocarbon fuels, increasing the efficiency of their use, and minimizing attendant pollution. A critical aspect of the combustion process requiring detailed understanding is that of extremely rapid chemical reactions. Molecular species exist in, and affect the course of, chemistry in a flame; among these are transient species known as molecular radicals. Their behavior in the flame is strongly affected by internal bond energies. These binding energies between atoms in a molecule are described by the thermodynamic quantity known as heat of formation. This quantity is very difficult, if not impossible, to measure for very short lived transient species. Thus, theoretical calculation of heats of formation is necessary.

Recently, a new theoretical approach has been developed which allows calculation of heats of formation with much greater reliability than before. Using this new approach, it has been shown that previously accepted values for heats of formation of the nitrogen-hydrogen radicals NH and NH_2 are not correct. Further, for the first time, the heats of formation of several other radicals made up of carbon, hydrogen and oxygen atoms have been determined. This new approach will help bring more order and insight to the understanding and exploitation of combustion processes, providing an important new tool for combustion chemists and engineers.

(Sandia National Laboratory-Livermore, Combustion Research Facility, C. Melius and S. Binkley)

23. <u>Balancing the Global Carbon Cycle Improved</u>

A considerable amount of research reported over the past year supports the fact a significant overall lowering of the estimated magnitude of release of both the historical and contemporary amounts of terrestrial carbon. For example, the net amount of carbon released because of contemporary changes in land use has been justifiably revised downward by a significant amount, from a range of 1.8 to 4.7 gigatons of carbon per year to 0.5 to 1.8 gigatons per year (a gigaton, equals 10^{15}g). This has greatly reduced the magnitude of the incompatibility between estimates of oceanic CO_2 uptake and terrestrial CO_2 release. Further, more recent estimates of early atmospheric CO_2 levels based on refined analyses of occluded air in early 19th century ice are 20 parts per million by volume (ppm) higher than values reported previously. The higher values are also more compatible with reduced estimated of terrestrial fluxes.

These new findings continue to suggest that the oceans may be assimilating more CO_2 from the atmosphere than has been estimated until now. Refinements in ocean carbon cycle models averaged for the entire Earth have resulted in estimates of the amount of CO_2 taken up by the oceans that are 25% higher than those established previously. However, current ocean models are still unable to accommodate a significant release of CO_2 from terrestrial ecosystems. Further progress toward balancing the carbon cycle depends on more realistic and geographically detailed models of both the oceanic and terrestrial carbon systems. Development of such models, in turn, depends on an enhanced data base of carbon reservoirs and fluxes in both time and space.

(Oak Ridge National Laboratory, L. Mann; Bern U., Switzerland, Hans Oescher; U. Of Illinois, S. Brown; U. of Puerto Rico, A. Lugo; Marine Biological Laboratory, R. A. Houghton, J. Melillo; Duke U., W. Schlesinger)

24. Photosynthesis Regulation

Photosynthesis, the energy process that provides food, fuel, and fiber for life on earth, is now conceived as having two light driven photosystems that are connected by a biochemical chain called the electron transport system. How the two photosystems are coordinately regulated has been a long standing question. Recent work has produced an explanation for this regulation. The mechanism involves the phosphorylation (adding phosphorous) to some key proteins (light harvesting chlorophyl and protein complex) in response to the oxidation-reduction state of one of the components of the electron transport chain. This mechanism of phosphorylation and de-phosphorylation of photosynthetic proteins affords a more balanced distribution of the trapped light energy between the two photosystems and consequently probably improves the overall efficiency of photosynthesis. The understanding of such control mechanisms is important to designing artificial light trapping devices and could enter into future plant improvement strategies intended to enhance plant (renewable) productivity.

(Brookhaven National Laboratory, J. Bennett)

25. Measurement Made of D-T Reaction to Much Higher Accuracy Than Ever Before

The basic fusion-energy reaction, deuteron + triton leading to alpha + neutron, has been measured to a much higher accuracy than ever before over a range of triton bombarding energies 12.5 to 117 keV, equivalent to plasma temperatures in the kT temperature range from 0.7 to 18.8 keV, This is the operating range of the first generation magnetic- and inertial-confined fusion reactors. The cross section is accurate to 1.4% over most of the energy range, with the error rising to 4.8% at the lowest energy. The measurement featured the use of a windowless, cryogenically pumped gas target, specially designed calorimeters to measure beam current, and special techniques to determine the target gas density. The system will be used to measure the cross sections for the reactions of other hydrogen and helium isotopes at the very low energies of interest to fusion technology and astrophysics.

(Los Alamos National Laboratory, N. Jarmie and R. E. Brown)

26. Increased Beam Intensity for Particle Accelerator Applications

Particle accelerators have been developed for a wide variety of applications, including basic research in high energy physics, nuclear physics, defense, and numerous industrial applications. In spite of decades of increasing both the beam kinetic energy and the beam intensity, the fundamental limits for the transport of intense beams in conventional transport systems have not been well known. Now, as a result of recent research conducted in the Heavy Ion Fusion Accelerator Research (HIFAR) program, these limits have been established. The HIFAR program, initiated to develop and evaluate heavy ion accelerators for inertial fusion energy applications, requires the maximum intensity possible to be successful. The program involves stages of research from single beam experiments to multiple beam accelerator development. A series of single beam experiments have recently been concluded which demonstrate that beam currents three times larger than previously thought possible are now feasible. These results apply not only to the HIFAR program but to a wide variety of other applications.

(Lawrence Berkeley Laboratory, D. Keefe and coworkers)

27. Chemical Purification of Uranium Aids in Isotopic Enrichment

A new concept has been discovered for improved cleanup of uranium hexafluoride (UF_6) gaseous process streams. These streams are central to recovering uranium from partially spent reactor fuel. The cleanup is necessary because certain products of the reactor fuel "burning" contaminate the UF_6 and interfere with the isotope enrichment process for uranium-235. Basic chemical studies found that gaseous metal fluoride impurities in the UF_6, such as neptunium hexafluoride, will react with solid uranium pentafluoride to form solid fluorides of the impurity metals. This removes the impurities from the gas stream. Later, the trapped impurities can be recovered photochemically for theiown value. The applicability of this cleanup procedure for removal of other metal contaminants is being examined.

(Argonne National Laboratory, J. V. Beitz)

28. A New Procedure in Stable Isotope Separation Better Serves Users' Needs

A new approach to operating the calutrons has led to simultaneous separation of isotopes of more than one element within a single magnetic segment. The calutrons are magnetic isotope separators that were built during the World War II Manhattan Project for the enrichment of uranium-235 but which are now used for the enrichment of many other isotopes for use in nuclear medicine, basic research, and industry. The need for a wide variety of isotopes for these applications is now being better met by this new procedure. While this new procedure separates a larger number of elements during a calutron run, it does however result in the production of smaller amounts of each isotope produced per unit of operating time.

(Oak Ridge National Laboratory, E. Newman)

29. Control of Actinide Valence States Important in Nuclear Waste Isolation

Thermodynamic studies have provided important guidelines for using synthetic mineral hosts for nuclear wastes. A candidate procedure for the disposal of the waste materials from the processing of nuclear fuels is to incorporate them into stable solid chemical compounds (hosts) that can be placed for long term storage in a repository. Such a compound could be mixed-metal oxide. To minimize escape of the radioactive wastes from the solid hosts into the ground water, both the hosts and the contained activities must be resistant to chemical degradation and solubility in water. Some of the important waste constituents are heavy actinide elements. It has been found that the plus-six valence state of the actinides is more leachable by water than the plus-four state and therefore the preparation of the solid host material must be carefully adjusted chemically to avoid the more soluble valence state of the actinides.

(Argonne National Laboratory, L. Morss)

30. Theory Challenged: Iron Oxide Clusters Maintain Fe_9O_{10} Ratio

As iron rusts, its atoms pass through more than one state of oxidation. The first of these stages is ferrous oxide, nominally made up of positively charged iron ions (Fe^{++}) and negatively charged oxygen ions (O^{--}) in a one-to-one ratio. But in nature the mineral ferrous oxide is found not to have this one-to-one ratio, having instead only 9 iron ions for every 10 oxygen ions. This has been thought to be due to a chemical action between pairs of iron ions, whereby some of the iron passes out of the mineral. Such behavior is understood in terms of a fully ionic structure, i.e., made up of only positively charged iron atoms and negatively charged oxygen atoms.

Now a new and clever technique has been devised by chemists at Argonne National Laboratory for study of the behavior of metal clusters containing only 2 to 60 metal atoms. Clusters of iron and oxygen atoms in that size range were believed to be unable to exist in a fully ionic structure, and thus unable to interact as described above for pairs of iron ions. The cluster should therefore maintain the one-to-one ratio of iron to oxygen atoms. To everyone's great surprise, what was found in clusters down to a size of 9 iron atoms was the same ratio as in the bulk mineral 9 iron to 10 oxygen atoms. These results demonstrate the need for a whole new approach to understanding the chemical and electronic structure of the iron oxides and, perhaps, of a much wider group of metal oxides. Since ferrous oxide and many other metal oxides are practical or potential semiconductors (transistors, computer chips), these results may lead to further studies having wide ranging benefits.

(Argonne National Laboratory, S. Riley and coworkers)

31. Microbial Population Changes in Anaerobic Digestors

Methanogenesis is a natural process that occurs in many ecosystems where oxygen is at very low levels (anaerobic). Man has harnessed methanogenesis in anaerobic digestors to produce methane gas which is used as a fuel. Despite the widespread occurrence and utilization of methanogenesis, the microbial ecology is still poorly understood. Two recent advances have begun to provide new insights into mechanisms of methanogenesis. During the course of the development of the microbial activity within an anaerobic digestor, it has been observed that the microbial populations change appreciably before stabilization is achieved. These dynamics have now been documented. Also, there has been the development of highly specific immunologic agents produced against various species of methanogenic bacteria which has made identifications easier, faster and more reliable.

With these findings and procedures available it may be expected that a better understanding of anaerobic digestion generally, and methanogenesis specifically, will proceed rapidly. These processes have important environmental implications as well as for the production of fuel, particularly in less developed countries.

(New York State Department of Health, A. J. L. Macario, E. Conway de Macario, and M. J. Wolin, and Cornell U., S. H. Zinder)

32. Electron-Molecule Interactions Important for Excimer Lasers Measured

A scientific breakthrough has been achieved which is important to laser developers. For the first time, absolute measurements have been made of the interaction of electrons with individual molecules which are electrically polar, that is, molecules in which electrons are displaced to produce poles, much like a bar magnet, except that the poles in the molecule are electrical, not magnetic. The previous inability, whether theory or experiment, to provide this kind of information has hampered the understanding and advancement of a class of lasers known as excimer lasers. Previous experimental efforts have been indirect, requiring researchers to rely on theory to interpret their results. But the theory itself has given ambiguous and conflicting results. Now, physicists have cleverly devised an experimental setup for direct measurement of the interaction. The setup involves a beam of cesium bromide vapor intersecting an electron beam. Following the encounters in the intersection of the beams, the emerging molecular ions, molecules and electrons were measured and their energies and angles of emergence determined. The results showed this particular interaction to be one of the longest range ever observed between a point charge and a neutral system (on the scale of molecular dimensions, of course). This achievement was followed up by similar measurements on other polar molecules. The measurements are sure to be used to improve greatly the physical theory of this type of interaction, and should contribute to the practical development of excimer lasers.

(New York University, B. Bederson and B. Jaduszliwer)

33. New Levels of High Static Pressure, 2.5 Mbar, Reached with an Advanced Diamond Anvil Cell

Development of a new design of a diamond anvil pressure cell has resulted in the attainment of a new record static high pressure of 2.5 Mbar (about 38 million psi). The key to the design is the achievement of very precise alignment of the diamond facets, full metal gaskets, and miniaturizing the sample size to about 30 microns in diameter. From initial experiments it appears that pressures as high as 3 Mbar will soon be reached and that the novel technique can be used for a wide class of sample materials, including hydrogen. In these initial experiments on a ruby chip, the ruby fluorescence line - the shift of which is presently used by high pressure scientists as a pressure scale - is lost above 2 - 2.5 Mbar suggesting the ruby itself has become metallic.

The achievement of a static pressure of 2.5 Mbar - almost twice that previously obtained - opens the way for the investigation of materials under extreme conditions and will aid in the search for new materials. An important example is the investigation of hydrogen at multi-Mbar pressures: recent theoretical studies indicate that hydrogen will become metallic at pressures between 3 and 4 Mbar and it is expected to have a very high superconducting transition temperature and a very high Debye temperature (a very hard material). Entirely new classes of materials with unusual and useful properties can be expected to result from research in the very high pressure regime.

(Carnegie Institution, P. Bell and H. K. Mao)

34. New Method for the Analysis of Experimental Nuclear Data

An innovative approach to the treatment of uncertainties associated with experimental data has been developed at ORNL and applied to the analysis of nuclear data. This new technique utilizes group-theoretical methods to treat in a coherent way both statistical and systematic uncertainties.

New approaches developed from this fundamental breakthrough have been implemented in computer programs designed to use well-understood resonance-interaction theory to accurately analyze many thousands of neutron-scattering data points. The complete set of experimental uncertainties, including correlations, is carried through all steps of the analysis, so that the deduced resonance parameters have uncertainties correctly determined from the original experimental uncertainties.

(Oak Ridge National Laboratory, F. G. Perey)

35. The Cosmic Cube, a 64 Processor Computer, is Operational

Researchers have successfully built a 64 processor research computer with the equivalent computing power of one-tenth a Cray-1 at one-hundredth the price. This architecture is dramatically different from today's Class VI machines and early results indicate it may be a cost effective alternative for a variety of scientific problems. The current machine located at California Institute of Technology, uses 64 processors with nearest neighbor or local interconnections amongst processors. It has long been realized that such machines could provide substantial speed up on computations where the interactions amongst objects being computed had a similar local structure; i.e., speed up would be possible if the topology linking the processors mirrored the topology linking the objects being computed. It has been demonstrated that speed ups on such problems were indeed possible, but more importantly, it has now been shown that a large class of problems with non-local interactions could be effectively mapped into ones with approximately local interactions which could then be solved effectively on the Cosmic Cube. A lattice gauge problem modeling fundamental properties of matter ran for 2500 hours on the cube and provided scientists with highly reliable and interesting results on the heavy quark potential. A variety of other problems have been implemented on this machine, including ones from astrophysics, molecular dynamics, geophysics, and critical phenomena in materials.

(California Institute of Technology, G. C. Fox and C. L. Seitz)

36. Capillarity Phenomenon Mathematically Predictable

It has been found that the solution of the equations governing liquid free surface interfaces predicts unexpected behavior if the cross-section of the tube is not circular. It was concluded that the solution of the equations can behave discontinuously or even cease to exist when small changes are made in contact or capillary-tube cross-section. For example, when applied to the case of a wetting liquid in a tube of square cross-section in zero gravity, analysis predicts that for contact angles greater than or equal to a critical value of 45 degrees the height of the free surface (portion of a sphere) is uniformly bounded, but for smaller contact angles no solution of the equation exists. This remarkable behavior was verified experimentally at the NASA-Lewis Research Center in their Zero Gravity Drop Tower. It was observed in tests that for contact angles less than the predicted value the fluid flowed up along the corners rather than remaining simply contained in the bottom of the tube. While these findings have intrinsic mathematical importance, they may find applications in such practical areas as flow in heat pipes, growth of crystals in low gravity, behavior of petroleum in underground reservoirs, and other areas in which capillarity phenomena play a role. The effect of zero-gravity capillarity is important in space manufacturing and will be investigated further in an upcoming space shuttle flight experiment.

(Lawrence Berkeley Laboratory, N. Albright et al; Stanford University, J. Marsden, A. Weinstein)