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Brookhaven Highlights

October 1979 September 1980

High Energy Physics

Physics and Chemistry

Life Sciences

Applied Energy Science

Support Activities

General and Administrative

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Introduction

Brookhaven National Laboratory is operated by Associated Universities, Inc. (AUI) under a contract with the United States Department of Energy (DOE). The Laboratory conducts a broad range of basic and applied research programs in the physical and life sciences. It occupies a 21 km^2 tract of land at Upton, NY, approximately at the geographic center of Long Island, about 100 kilometers east of New York City.

AUI was formed in 1946 by a group of nine universities for the purpose of establishing and managing Brookhaven National Laboratory and other research centers. This action represented a new approach to the management of fundamental research with the support of the Federal government, especially for large-scale scientific enterprises of importance to the academic community.

From 1947 to 1975 the Laboratory was supported by the U.S. Atomic Energy Commission. In 1975 the Atomic Energy Commission was abolished, and most of its research programs were taken over by the Energy Research and Development Administration, which in 1977 was incorporated into the newly created Department of Energy. The U.S. Nuclear Regulatory Commission, which was formed in 1975 to take over the regulatory functions of the AEC, supports a continuing program of studies at Brookhaven on the safety of nuclear power reactors.

The primary objectives of the Laboratory are:

— To seek new scientific knowledge, with emphasis on programs that require large-scale research tools such as particle acclerators, nuclear reactors, and special laboratories that are beyond the scope of individual educational institutions.

— To encourage use of its facilities by scientists from universities, research institutions, and industry.

— To assist the Department of Energy (DOE) in the performance of tasks that utilize the Laboratory's unique facilities and organization or the special talents of its staff.

— To serve as an important auxiliary in the training of scientists and engineers, and otherwise to assist in the dissemination of scientific and technical knowledge.

To fulfill the first and second of these objectives, the Laboratory has designed and built a series of large research devices. The first generation of these, the Cosmotron and the Brookhaven Graphite Research Reactor, have already completed long and useful programs of research and have been replaced by newer machines. Today the Alternating Gradient Synchrotron (AGS) accelerates protons to energies up to 30 GeV and continues as one of the nation's pri mary devices for high energy physics research. The High Flux Beam Reactor provides intense beams of neutrons for fundamental experiments in nuclear and solid state physics, chemistry, and biology. The Medical Research Reactor serves for activation analyses and for medical dosimetry studies. The Tandem Van de Graaff installation provides beams of many varieties of ions at energies up to several hundred MeV for fundamental research in nuclear physics. Several smaller accelerators are also employed for solid state physics and nuclear research. A 60-inch cyclotron and the linac injector to the AGS produce many special isotopes, primarily for medical research and treatment. A scanning transmission electron microscope provides extremely high resolution for investigation of biological molecules and subcellular structures. A pulmonary toxicology facility allows the study of animals exposed to atmospheres of hazardous substances.

In each of these facilities a core of Brookhaven scientists and engineers performs research and oversees the maintenance and upgrading of the facility. Scientists from universities, other laboratories, and industry also use the facilities, sometimes in collaboration, and often independently. At many of the facilities the visitors outnumber the Brookhaven users substantially. At the AGS, for example, about 80% of the research is done by visitors.

In furtherance of this role of providing research machines, the Laboratory has under construction two new devices designed to meet developing needs of science: The ISABELLE colliding beam storage accelerator will provide intersecting beams of protons at energies up to 800 GeV in the center of mass system (equivalent to protons impinging on a fixed target with energy of 340 TeV). This machine will allow deeper studies into the nature of matter and the fundamental forces which hold it together. The National Synchrotron Light Source will provide intense beams of ultraviolet light and x-rays for experiments in physics, chemistry, the life sciences, and technology.

The third of the Laboratory's primary objectives has resulted in the formation of selected programs in energy technology and in various kinds of technical support to the Department of Energy. Included are programs to apply superconductivity to the transmission of large blocks of electric power; to develop intense sources of negative ions for heating plasmas for fusion; to develop a new method for the flash hydropyrolysis of coal; and to develop better electrochemical systems for energy conversion and storage. Technical support to the DOE is provided by the National Center for Analysis of Energy Systems, which conducts a variety of national and regional studies on energy systems, their characteristics, and their impacts on health; the Technical Support Office for Safeguards, which analyzes systems for preventing the diversion of fissionable materials to unauthorized uses; and the National Nuclear Data Center which assembles and disseminates data on the properties of atomic nuclei.

It should also be emphasized that the Laboratory's programs in nuclear, atomic, and solid state sciences, in chemistry, and in applied mathematics are designed to help create a technology base for the entire energy program of the DOE. These and the various applied programs build on the strengths and unique facilities of the Laboratory, utilizing its special character, particularly its devotion to frontier science, its close coupling to the academic community, and its experience in working with industry. The contributions are vigorous, broad, and effective.

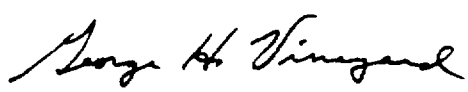
The Laboratory's objective of training is accomplished primarily through the provision of research opportunities for students from colleges and universities. The Laboratory is not a degree-granting institution, but helps such institutions through its research facilities. Students and faculty come to the Laboratory throughout the year and particularly in the summer, not only to use the unique devices but as participants in all of the Laboratory's research programs. In addition, numerous conferences in sciences and technology are sponsored by Brookhaven. Developments of technological significance made at the Laboratory are expected to be passed on to industry for commercialization, and an increasing effort is being made to this end.

This issue of the HIGHLIGHTS covers the Fiscal Year 1980, i.e.,the period from October 1979 through September 1980.

Since the special facilities are best seen in terms of the research that is done with them, the arrangement of the last HIGHLIGHTS has been followed, in which major additional facilities or improvements to existing ones are linked to the research program of the department that is the principal user. Thus ISABELLE is described in the High Energy Physics section, and the National Synchrotron Light Source, due for completion in 1981, is described after the program of the Physics Department.

In the hope of making things easier for readers who wish to know more about particular items, references to selected published papers and staff lists with indication of individuals' particular interest have been appended. The comments of readers would be most welcome.

Finally, the editorial work of Dr. J. B. Horner Kuper on this report is gratefully acknowledged.



George H. Vineyard
Director

High Energy Physics

High Energy Physics Research

Accelerator Department

ISABELLE

Accelerator and High Energy Physics Programs

General Introduction

The high energy physics program is the largest single item in the Laboratory budget. This is a comprehensive program of experimental and theoretical research into the ultimate nature of matter. At present, the experimental program centers around the Alternating Gradient Synchrotron (AGS), which accelerates protons to an energy of 30 billion electron volts (GeV). Beams of these protons, or secondary particles produced by them, are used as projectiles to explore sub-nuclear matter. By studying the way in which the projectile particles interact with target particles inside an atomic nucleus, much can be learned about the kinds of constituents which make up sub-nuclear matter and about the forces which govern their interactions. At present it appears that the neutrons and protons which make up atomic nuclei are themselves formed of more fundamental entities called quarks which are bound together by gluons, special particles which transmit the strong force. Many other particles are produced in high energy scattering experiments and these are also believed to be composed of various combinations of quarks held together by gluons. All together there are perhaps half a dozen quarks and a similar number of leptons (an equally fundamental class of particles of which a familiar example is the electron). This modest number of quarks and leptons plus their antiparticles and a few force-carrying particles such as the gluon are thought to explain all of the rich variety of matter. This model of the physical world has had outstanding success but there remain many questions and puzzles. Not all of these particles have yet been observed and not all of the observed ones are fully understood.

It is the aim of the Brookhaven High Energy Physics program to investigate these most fundamental questions and to provide a center where scientists from other institutions can use the most powerful research tools available for this purpose.

ISABELLE, BNL's new high energy intersecting storage accelerator now under construction, will achieve collision energies about 100 times as great as those of the AGS. Many of the present puzzles in particle physics theory should be solved by the results of experiments using ISABELLE.

Proposals for experiments using the AGS must be submitted to the High Energy Advisory Committee which is composed of highly qualified physicists representative of the entire user community. This committee advises the Deputy Director for High Energy Physics who must approve all experiments before they can be scheduled on the AGS. About 80% of the research is carried out by visiting scientists from universities, other national laboratories, and occasionally from abroad.

The Accelerator Department operates the AGS and its experimental areas, providing the beams of protons, antiprotons, kaons, mesons, and neutrinos which are needed for experiments. Department personnel assist the experimenters in setting up their apparatus and provide many services essential to carrying out experiments. Large facilities, such as the Multiparticle Spectrometer and the On-Line Data Facility, are constructed, operated, and maintained by the Department. Some of the Department physicists also participate in research.

The Physics Department is staffed with both experimentalists and theorists. The experimentalists are mainly involved with research at the AGS, but a small fraction of the effort is carried out at other accelerators. The theorists provide the stimulus of exciting new ideas in particle physics and devote much of their time to a study of results from experiments using the AGS and other high energy accelerators in the U.S. and Europe.

The High Energy Discussion Group (HEDG) is an organization brought into being by the community of university and national laboratory users of the AGS "to provide an organized channel for the interchange of information between those who utilize BNL high energy facilities for their research and the Laboratory administration." HEDG holds one general meeting at BNL every spring. Much of the work of the users group is coordinated by the HEDG Executive Committee which meets three times a year.

High Energy Physics Research

INTRODUCTION

Experimental and theoretical research in high energy physics at Brookhaven is carried out by members of the Physics Department, often working in collaboration with members of the Accelerator Department and physicists from outside institutions, primarily universities. Members of the Physics Department staff engaged in this research are listed beginning on page 57.

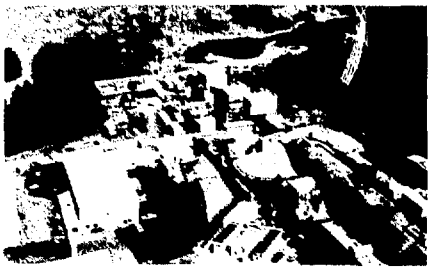
The discovery of the J/ψ particle at BNL and SLAC in 1974 led to a revolution in high energy physics. Previously, the spectroscopy of established resonances was well described in terms of a substructure of three particles called "u", "d", and "s" quarks. The various types of interactions of particles are usually classified into four categories: strong interactions which supply the force to hold nuclei together, electromagnetic interactions, which hold atoms together, weak interactions which manifest themselves in radioactive decays, and gravitation, which determines the motion of planets. (Particles which can undergo strong, electromagnetic, gravitational, and weak interactions are called hadrons while the particles which can undergo only electromagnetic, gravitational, and weak interactions are called leptons). This proliferation of "forces" is inelegant and much effort has gone into a more general description. In 1967, Weinberg and Salam suggested a gauge theory that combined electromagnetic and weak interactions. The theory with just three quarks was not able to explain certain other experimental results. However, it was shown in 1970 by Glashow, Illioupoulis, and Maiani that the introduction of a fourth quark, "c", could overcome these difficulties. This quark, which had been postulated earlier, leads to the existence of a whole new spectrum of high mass, relatively long-lived resonances. Such a spectrum has been confirmed (J/ψ being the first evidence for the c quark) and the success of the prediction has led to great confidence in the whole idea of gauge theories, which were recently further buoyed by the discovery of a fifth quark, "b," at Fermilab.

Currently, the most popular theory of strong interactions, also a gauge theory, is "quantum chromodynamics" (QCD). In addition to quarks, this theory contains "gluons" (g) which provide the force to hold the quarks together. QCD predicts multigluon and quark-gluon resonances at relatively low mass as well as the normal multi-quark resonances. Searches for these new particles, and the general study of hadronic production of resonances, are well-suited for BNL, since the beam energy required is within the range of the AGS, and the complicated apparatus needed for such experiments is available.

Much attention is now being given to "Grand Unification" theories, which bring strong interactions into the fold, combining them with electromagnetic and weak interactions into a single gauge theory. Startling predictions are already apparent, including possible decay of the proton, previously considered stable.

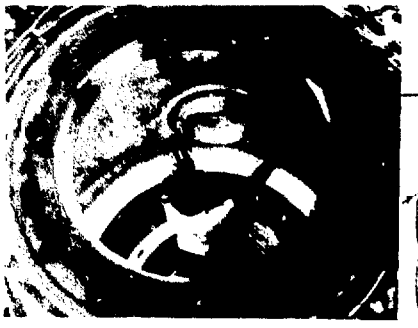
OVERVIEW OF AGS EXPERIMENTS

Most of the BNL high energy physics research uses the Alternating Gradient Synchrotron, which produces a beam of 30 GeV protons. When the protons are allowed to strike a target many kinds of subatomic particles are produced, including pions, kaons, and antiprotons. Some experiments use the primary proton beam, but most study the interactions of these secondary particles. In this case, the secondary particles are focused on a target (usually liquid hydrogen, the simplest element) using magnetic lenses. Tracking detectors then measure the various outgoing particles to investigate the nature of the interactions. Another type of experiment observes the decay of unstable beam particles (usually kaons) in the study of weak interactions. A third type of experiment focuses the charged particles, but then allows a long flight path along which many unstable particles decay, leading to a beam of neutrinos and

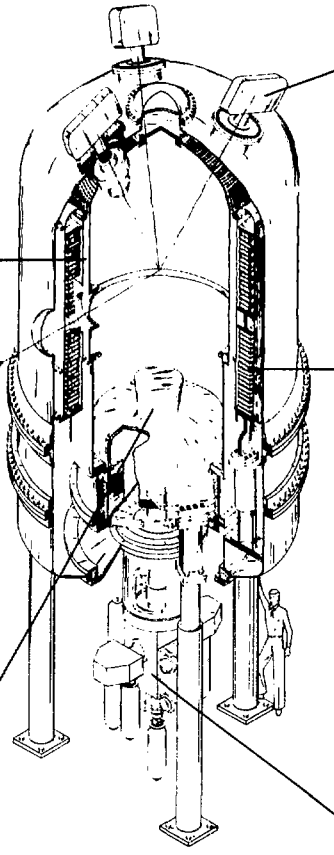


7-Foot Bubble Chamber

Film Transport



Installing Scotchlite



Superconducting Magnet

Piston

Hydraulic Expansion System

Figure 1. The BNL 7-foot bubble chamber. A cut-away sketch illustrates the overall layout and the photographs show various components. The bubble chamber was shut down in 1980 after many years of service in the study of neutrino interactions.

other decay products. A thick shield is then used to absorb all particles except the neutrinos, which pass through it to the detectors. These three classes of experiments will be discussed separately.

NEUTRINO EXPERIMENTS

The concept of the neutrino, a lepton postulated to have zero mass and charge, was introduced in the 1930's in order to explain the continuous nature of the β decay spectrum. The electron neutrino, ν_e, was detected at Savannah River in 1956 and it was demonstrated at BNL in 1962 that the muon neutrino, ν_μ, is a different particle. It is also expected that a third neutrino, ν_τ, associated with the τ lepton discovered at SLAC in 1975, will turn out to be a distinct particle. The theory of weak interactions which has been very successful and widely accepted since the late 1950's, assumes that the neutrino mass is exactly zero. The new grand unified theories now suggest a finite mass. The experimental limits on neutrino mass in the 1978 Review of Particle Properties were $\nu_e < 60$ eV, $\nu_\mu < 6 \times 10^5$ eV, and $\nu_\tau < 6 \times 10^8$ eV, leaving plenty of room for neutrinos with mass. Indeed, a recent experiment at ITEP (USSR) examined the β decay spectrum of tritium and reported a ν_e mass in the region 14 to 46 eV. If one allows for non-zero neutrino masses, the possibility arises that neutrinos may oscillate from one type to another, at a rate proportional to the difference of the squares of the masses of the neutrinos involved (Δm^2). Recent data taken at the Savannah River reactor indicate that, indeed, ν_e's might be changing into ν_μ or ν_τ, although the statistics are not overwhelming. Analysis of the data suggests $\Delta m^2 \sim 1\ eV^2$, clearly consistent with the direct measurements of neutrino masses.

The question of neutrino oscillations has been studied in two experiments at BNL. One experiment used a large electronic detector to search for $\nu_\mu \rightarrow \nu_e$ oscillations. In such experiments one has to contend with a transition rate which is inversely proportional to the momentum of the neutrino. In order to reduce the neutrino momentum, and also to ensure a ν_μ beam (from π decays) with little ν_e contamination (from K decays), the AGS was operated at 1.5 GeV/c, where very few kaons are produced. The analysis of the data is in the final stages, with an expected sensitivity of $\Delta m < 1\ eV^2$. The second experiment used data from the FNAL 15-foot Bubble Chamber to search for oscillations of the type $\nu_\mu \rightarrow \nu_e$ and $\nu_\mu \rightarrow \nu_\tau$. No events have yet been seen and the final sensitivity is expected to be $\sim 1\ eV^2$ for $\nu_\mu \rightarrow \nu_e$ and $\sim 3\ eV^2$ for $\nu_\mu \rightarrow \nu_\tau$.

The final run of the BNL 7-foot Bubble Chamber, Fig. 1, took place this year, bringing to an end an illustrious era of bubble chamber operation at BNL. For more than two decades these chambers were used in detailed studies of strange particles, hadron resonances, and neutrino interactions, highlighted by the discovery of the Ω^- particle and the first observation of charmed baryons. However, bubble chamber physics is still being pursued at BNL. Using pictures taken with the 7-foot chamber, about ten thousand neutrino interactions will be obtained, leading to very detailed studies of quasi-elastic scattering, strange particle production, etc. In addition a series of experiments using the FNAL 15-foot bubble chamber is continuing, with emphasis on charm production and careful studies of neutrino-nucleon interactions at high energy.

Meanwhile, the emphasis at BNL has shifted to counter techniques for detailed studies of neutrino interactions. An experiment to measure neutrino-electron scattering is being constructed. The main attraction of ν-e scattering is the simple interpretation of the data; the process is unencumbered by form factors caused by the presence of nucleons. It should yield the best determination of the Weinberg angle since the statistical errors will be better than other experiments and the systematic uncertainties will be smaller. The cross section for ν-e scattering is extremely small — at 1 GeV neutrino energy it is about $10^{-42} cm^2$, about 1/400 of that for ν-p elastic scattering (and 10^{-16} times typical hadronic strong-interaction cross sections!). Clearly, intense beams and a very large target are of the utmost importance, along with extremely good background rejection. Judicious spacing of large numbers of proportional drift tubes and liquid scintillator counters (which also serve as the target) leads to a background level comparable to that achieved in bubble chamber experiments, while the number of events will be an order of magnitude higher. A photograph of the partially completed experiment is shown in Fig. 2. When completed, the

Figure 2. A view of the apparatus to be used in the study of ν-e scattering. When completed, the apparatus will measure 4.27 m × 4.27 m × 22.9 m long with a total weight of 180 tons (metric). Electronic detectors are employed to identify particles and measure their energies and directions.

detector will use about 150 tons of liquid scintillator, 4,000 photomultiplier tubes, and 15,000 proportional drift tubes.

HADRON SPECTROSCOPY AND DYNAMICS

In addition to the standard mesons and baryons, the existence of a whole spectrum of multi-quark "exotic" mesons is expected. Particular attention has been paid to possible meson resonances, just above threshold in the $\bar{p}p$ system, known as baryonium. Several years ago a CERN experiment observed narrow peaks in the $\bar{p}p$ effective mass at 2.02 and 2.20 GeV/c^2 in the reaction

$$\pi^- p \rightarrow (p\pi^-)_{\text{forward}}(\bar{p}p).$$

Three experiments run at the BNL Multiparticle Spectrometer Facility, a large magnetic

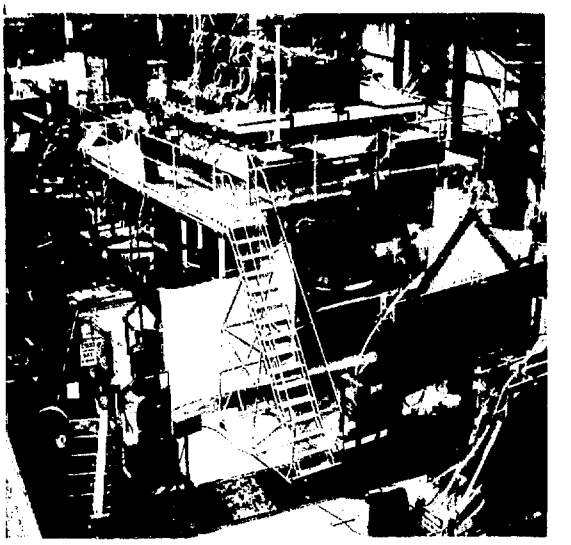


Figure 3. The BNL Multiparticle Spectrometer consists of a large electromagnet with poles 1.83 m × 4.57 m and a 1.22 m high gap. Digitized spark chambers and proportional wire chambers in the 10 kG magnetic field detect particles produced in high energy reactions. The spectrometer is currently being upgraded, with drift chambers replacing the spark chambers, leading to experiments an order of magnitude more sensitive.

spectrometer with electronic detectors (see Fig. 3), were designed to study these and related resonances. One used the same reaction as the CERN experiment, and another studied the related reaction

$$\pi^+ p \rightarrow (p\pi^+)_{\text{forward}}(\bar{p}p).$$

The results, which are shown in Fig. 4, disagree with the original experiment. The third experiment studies the reactions $\bar{p}p \rightarrow \bar{p}p\pi^0$ and $\bar{p}p \rightarrow \bar{p}p\rho^0$, again with a negative result. Thus all three experiments, rather than extending the spectroscopy, found no indication of any bump. It seems that the original experiment was plagued by large statistical fluctuations. A similar fate has befallen another baryonium candidate: a large bump observed earlier in the $\bar{p}p$ total cross section at an effective mass of 1.936 GeV/c^2 was not seen in recent experiments at BNL which studied total cross sections, annihilation cross sections, backward elastic scattering, and charge exchange scattering. One has to conclude that the earlier experi-

ments were incorrect, although the study of possible effects at a lower cross section level is being pursued. These episodes illustrate the importance of maintaining good facilities so that exciting, or controversial, experiments can be checked independently; otherwise, progress in the field can be hindered by the four or five standard deviation fluctuations that occur occasionally.

One of the most controversial members of the "charmonium" ($c\bar{c}$) family of resonances is the η_c, which is expected to be slightly lower in mass than the J/ψ. Early candidates were observed at the e^+e^- storage ring at DESY (Hamburg) and in π^- induced reactions at Serpukhov (USSR) at a mass of ~2.8 GeV/c^2. However, the theory of $c\bar{c}$ states, which fitted the rest of the spectrum very well, was hard-pressed to accommodate a mass this low. A more recent candidate with a mass of 2.90 GeV/c^2 has been observed at SLAC, but confirmation is needed. A search was conducted at BNL in the reaction

$$\pi^- p \rightarrow \eta_c n$$
$$\hookrightarrow \gamma\gamma$$

using a pair of large, high resolution, lead glass hodoscopes to detect the two γ-rays. A short run was analyzed in 1980; no two-γ events were

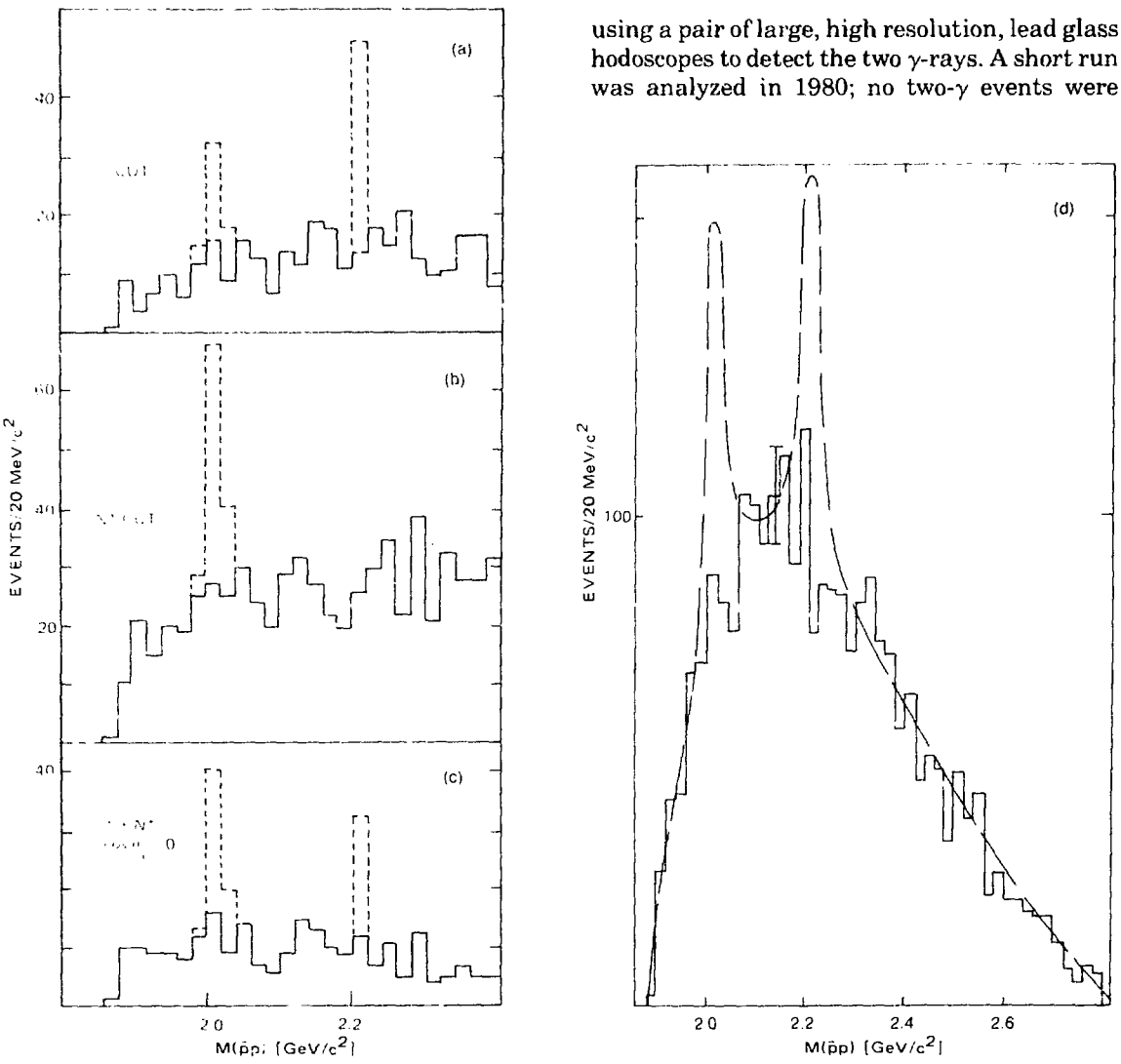


Figure 4. (a) (b) (c) the $\bar{p}p$ effective mass spectrum for the reaction $\pi^- p \rightarrow (\pi^- p)_{\text{forward}} \bar{p}p$. The dashed lines show the signal expected on the basis of earlier experiments. No signal is seen. (d) The $\bar{p}p$ effective mass spectrum from the reaction $\pi^- p \rightarrow (\pi^- p)_{\text{forward}} \bar{p}p$. The dashed curve shows the expected spectrum. No peaks are seen.

observed at an effective mass above 2.2 GeV/c^2 and the limits for particles at 2.8 GeV/c^2 are low enough to cast great doubt on the earlier measurements at Serpukhov. The main run was completed in 1980 and will have two orders of magnitude higher sensitivity.

The spectroscopy of conventional hadronic resonances is still relatively incomplete; just a few of the families of resonances predicted by QCD have been completely explored, leading to great difficulty in the disentangling of new phenomena, such as "glueballs" (gg, ggg, etc.). An experiment was performed in the BNL Multiparticle Spectrometer using the reaction $\pi^- p \rightarrow K_S^0 K_S^0 n$, to study resonances in the $K_S^0 K_S^0$ system, which is restricted by symmetry to have $J^P = 0^+$, 2^+, 4^+, etc. An earlier test run yielded 3,000 events (which is comparable to the number in earlier experiments) and showed the expected structure corresponding to known resonances. The data from the full run are being analyzed, with a final sample of about 30,000 events expected. Detailed analysis of the angular correlations is proceeding, with expectation of new contributions to the spectroscopy of hadrons.

As has been the practice over the years, a small fraction of BNL high energy physics research takes place at other laboratories in order to take advantage of the full energy range available to experiments. One collaboration is at the CERN Intersecting Storage Ring, the only pp storage ring in operation. Several high resolution liquid-argon calorimeters which can separate electrons, π^0's, and single γ rays, are placed at 90° to the beam axis. Single γ rays have been clearly separated and studies of the hadrons produced along with these photons are proceeding. Meanwhile, the construction of a large magnetic spectrometer, with uranium calorimeters, is under way, with initial plans to study high momentum transfer events containing jets and individual hadrons. This work will be very valuable in planning experiments for ISABELLE.

Weak Decays of Hadrons

The 1980 Nobel Prize for Physics was awarded to V. L. Fitch and J. W. Cronin for their discovery at BNL in 1964 of violation of time-reversal invariance (T) in K° decays. Since the original discovery, many experiments have studied the nature of the violation, with little success in establishing the mechanism at work. An experiment performed at BNL last year measured the polarization of muons from the decay $K^0 \rightarrow \mu^+ \pi^- \nu$. If T is conserved in this decay, the muons can be polarized, but the polarization must lie in the plane of the decay (apart from a small correction due to electromagnetic interactions between the μ^+ and π^-). The result, though more than twice as accurate as earlier measurements, was consistent with no T violation. Unfortunately, the precision was not quite enough to distinguish between the two main candidates for the theory of T violation, one of which predicts effects just below the limits of the experiment. The electromagnetic effects mentioned above also come in at about this level, so further studies will be pursued in another experiment to study $K^+ \rightarrow \mu^+ \pi^0 \nu$, where the presence of only one charged particle in the final state removes the electromagnetic corrections. Running started during 1980.

The family of baryons is made up of particles of half integral spin (1/2, 3/2, etc.) which undergo strong interactions. The two most familiar are the neutron and the proton, which account for most of the mass of atoms. It is generally assumed that "baryon number" (neutrons and protons have baryon number +1, antineutrons and antiprotons have baryon number −1, for example) is conserved in all interactions. If so, then the lightest baryon, the proton, is stable, unlike the neutron which undergoes β decay to the proton in the decay scheme $n \rightarrow p + e^- + \nu$ (one should note that the β^+ decay of nuclei, which leads to the transformation of a proton to a neutron, is permitted by the details of the energy balance of neutrons and protons bound in nuclei, and still conserves baryon number). However, conservation of baryon number is an experimental statement, with current lower limits for the lifetime of the proton of about 10^{30} years, some 10^{20} times longer than the estimated lifetime of the universe! Recently, interest in measurements of the proton lifetime have been revived by theories of grand unification of strong, electromagnetic, and weak forces, many of which predict proton lifetimes of around 10^{32} years. Clearly, if one expects to detect such rare decays, many protons must be observed simultaneously. BNL is collaborating in an experiment to detect proton decay in a large tank containing 10,000 tons of water, or about 10^{34} nucleons, giving 10 decays a year if the lifetime is 10^{33} years. The experiment will take place in

a salt mine 600 meters underground; this is sufficiently deep to reduce the background from cosmic ray muons to a manageable level. The most serious background at this point is due to the interactions of cosmic ray neutrinos which limit the sensitivity to about 10^{33} years. The experiment is currently being set up and should produce results in the next few years. A negative result will spur the consideration of performing the experiment on the moon, since the limiting background of neutrinos comes from the interaction of cosmic rays in the earth's atmosphere!

HIGH ENERGY THEORY

Significant progress was made by the High Energy Theory Group on a wide variety of problems. These range from the most fundamental studies of solutions of Yang-Mills equations and quark confinement, through phenomenological studies of jets and charmed particle decays, to studies in support of the design of experiments at ISABELLE.

A major effort has been devoted to the application of Monte-Carlo methods to non-Abelian gauge theories formulated on a space-time lattice. Monte Carlo simulation of statistical systems is a familiar tool of the condensed matter physicist. Quite recently, however, particle theorists have applied this technique to quantum field-theory, and in particular to the study of quark confinement in four dimensional gauge theories. This use of statistical methods has been made possible through Wilson's formulation of gauge fields on a space-time lattice. The primary virtue of this discrete treatment of space is the non-perturbative removal of the divergence rampant in quantum field theory. The lattice is a mathematical trick for defining the theory; at the end of a calculation the continuum limit of vanishing lattice spacing must be considered. Once formulated on a lattice, a gauge theory is equivalent to a statistical mechanics problem. In this analogy, temperature corresponds to the square of the unrenormalized field theoretical coupling constant. In his original paper, Wilson studied a high temperature expansion and found that quark confinement arose naturally. However, for the continuum limit of interest to particle physics, the temperature must be taken to zero. To show the persistence of confinement into this region, it would be simplest if no phase transition occurred in the equivalent statistical system. Brookhaven has an ongoing research program to investigate this system with Monte Carlo simulation techniques. The gauge fields are stored in the computer memory and then randomly varied in such a manner as to produce a configuration typical of "thermal equilibrium." The properties of this "vacuum" state can then be studied. As hoped, strong evidence against a deconfining phase transition has accumulated for the gauge groups SU(2) and SU(3). By contrast, in other models, such as the U(1) gauge group of electrodynamics, where confinement should break down, clear singularities appear as the "temperature" is varied. Recent work has centered on obtaining physical predictions from this analysis. For pure gauge fields, the strength of the long-range interquark force has been calculated in units of the scale parameter characterizing the short-range logarithmic decrease of the effective renormalized coupling constant. This represents a truly non-perturbative calculation of a parameter relating opposite extremes of length scale. Current attempts are being made to extract a mass for the first bound state of pure gauge fields. The limitations of the Monte Carlo method are far from being mapped out; this research will continue to occupy the theory group for some time to come.

Studies were pursued of the experimental consequences of perturbative QCD. In e^+e^- annihilation the interaction is pictured in terms of intermediate states consisting of quarks and gluons, which then materialize into observable jets of hadrons; the study of these jets will provide important information about the underlying dynamics. The influence of quark and gluon masses on the hadron distribution was calculated, and shown to be substantial at energies presently available at PETRA. An upper limit of 800 MeV for the gluon mass was obtained (in QCD the gluon mass is predicted to be zero). The inclusive production of heavy $q\bar{q}$ states in e^+e^- annihilation was also examined in perturbative QCD, in order to predict the details of the jet structure. Quark diagrams for the decays of various mesons containing c and b quarks were studied, with particular emphasis on the effect of flavor-changing neutral currents and CP violation. An analysis of the effects of the weak decays of heavy quarks in $q\bar{q}$ systems has shown

that the dilepton branching ratio is substantially reduced for $q\bar{q}$ mass greater than about twice the W mass. Hence the dilepton decay mode, which was a dramatic signal in the case of the $c\bar{c}$ (J/ψ, etc.) and $b\bar{b}$ vector mesons, may not be useful for more massive $q\bar{q}$ states.

A striking prediction of grand unification theories is the decay of the free proton. However, experiments to search for non-conservation of baryon number do not use pure hydrogen, but will look for the decay of nucleons bound in nuclei. It is important, therefore, to evaluate the effects of nuclear binding. Calculations show that changes in the total decay rate and in the resulting lepton momentum spectrum are not large, although the size of the correction is sensitive to the short distance internucleon wave function.

Accelerator Department

INTRODUCTION

The Accelerator Department is responsible for the operation of the major high energy facilities at Brookhaven, principally the Alternating Gradient Synchrotron (AGS).

In the AGS, protons are accelerated to high energies, then extracted and steered towards metal targets, where they interact and produce many secondary particles. These particles are focused into beams and transported by systems of magnets to areas where they are used to perform particle physics experiments. The Department oversees the scheduling of these experiments and provides services to user groups such as on-line computing, help with setting up heavy apparatus, and the use of large experimental facilities such as the Multiparticle Spectrometer (MPS).

Other work within the Department includes neutral beam development and superconducting power transmission.

The AGS

To begin the acceleration process, protons are produced by passing an electrical discharge through hydrogen gas. The protons are collected and made to enter a Cockcroft-Walton preinjector where they are accelerated to 750 keV. They are then accelerated in a 200-MeV linear accelerator (linac) and injected into the AGS.

The AGS is a proton synchrotron of the alternating-gradient type. The basic element of a synchrotron is the ring of magnets which guides the protons around an approximately circular path, and also applies a restoring force to particles which leave the central orbit. In the AGS, the shape of the magnetic field is reversed (alternating gradient) many times around the ring. This provides the strong focusing necessary to keep the beam confined to a small central region, which is important since the beam circulates entirely within an evacuated beam pipe lodged in the magnet gaps. While traveling in their almost circular trajectories, the protons are accelerated in rf cavities, located at several points around the ring, up to an energy of 29 GeV. They are then ejected from the main ring and sent down beam lines to target stations where they can be used by the experimenters.

Since the extracted proton beam is often split among several experiments simultaneously, it is desirable to achieve the highest possible intensity. The standard intensity is now more than 0.9×10^{13} protons/pulse while an intensity averaging over 10^{13} for an eight-hour shift has been achieved. The record peak intensity is 1.117×10^{13} protons/pulse. Figures 1 and 2 give the accumulated total protons accelerated and the total hours available for doing high energy physics experiments for the past several years. As can be seen in Fig. 1, 4.8×10^{19} protons were accelerated in FY 1980 (the period covered by this report), a 6.7% increase over FY 1979. The operating efficiency, defined as the ratio of total high energy physics hours over the sum of physics beam hours and unscheduled downtime, was 72.8% in FY 1980. For 26 weeks of operation the average number of high energy physics hours available per week was 132.8. The average intensity per pulse in FY 1980 was 0.67×10^{13} protons/pulse; this includes the periods when the machine was purposely detuned to meet certain experimental demands.

There are two extraction modes at the AGS. In the slowly-extracted-beam mode (SEB) the circulating beam is first debunched and then slowly extracted over many turns. This is accomplished by gradually "shaving" off some of the beam particles with an electrostatic septum, and then directing them to external beam lines by means of bending magnets. The whole

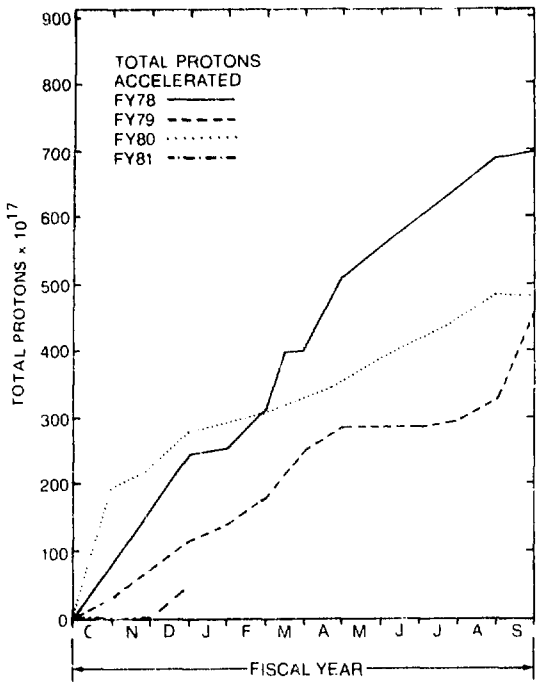


Figure 1. The total number of protons accelerated since the beginning of the fiscal year for FY 80, compared with FY 78 and FY 79.

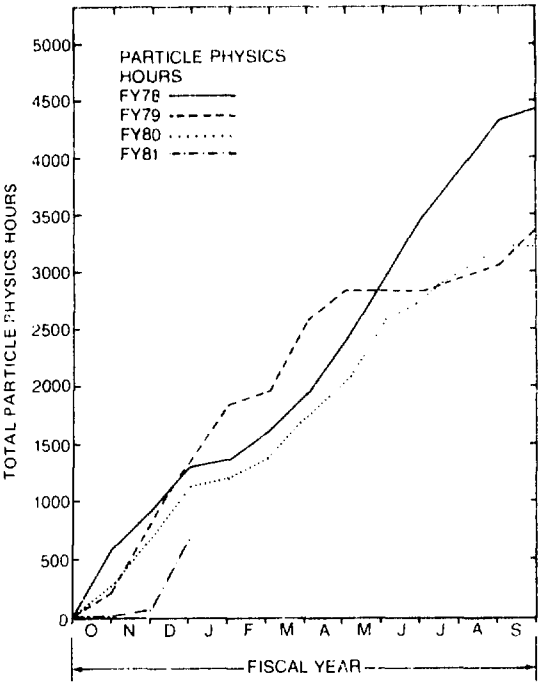


Figure 2. The total number of hours available for doing high energy physics experiments since the beginning of the fiscal year for FY 80, compared with FY 78 and FY 79.

beam is extracted in this way in the course of about one second. This relatively long time allows experimenters to take data smoothly without overloading their detectors. The total cycle requires about 2.5 seconds. The extracted beam is carried from the AGS ring to the targets via the SEB "Switchyard". This arrangement of beam splitting and transporting channels, which was commissioned in the prior fiscal year, has continued to perform with high efficiency and reliability this fiscal year. For neutrino experiments, where the interaction rates are much smaller, it is desirable to receive the full beam over a short period. In the fast-extracted-beam mode (FEB), the proton beam is not debunched, and is fully extracted in only one turn. In this case, the beam pulse is delivered within a few microseconds. Because the beam is extracted in a single turn, no "flat-top" is included in the magnet cycle, allowing a faster repetition rate (once every 1.5 sec). This yields more protons per week. During FY 1980, an experiment studying neutrino oscillation required beam at 1.5 GeV/c, resulting in a further shortening of the cycle. For this run, a repetition period of 0.8 sec was possible, resulting in a new record of 2.1×10^{19} protons in a 450 hour period.

In addition, the 200 MeV linac (which injects into the AGS) was extensively used by the Brookhaven Linear Isotope Producer (BLIP), the Chemistry Linac Irradiation Facility (CLIF), and the Medical Proton Radiogram Facility. The total 200 MeV proton flux delivered to BLIP in FY 1980 was 0.13 ampere hours, 20% more than for FY 1979.

IMPROVEMENTS TO THE AGS

H^- Injection

By injecting negative hydrogen ions into the AGS and stripping the electrons in a thin carbon foil inside the ring, a source of protons is created in the desired area of phase space (i.e., the desired ranges of position and velocity) for the duration of the injection pulse. Thus, all the protons are "overlaid" in the same phase space rather than "stacked" in adjacent phase space areas. This approach offers the possibility of

providing a brighter beam for ISABELLE injection. Other benefits should accrue from the high efficiency of injection (estimated as high as 98%) compared to 25% utilization of linac beam at present. This should result in greatly reduced radiation levels in the injection area and allow the peak linac intensity to be reduced, lessening the burden on the expensive rf power amplifier tubes and improving reliability.

Tests of an H source have been completed and are very encouraging. The source and its associated power supplies and controls behaved reliably. Measurements confirmed the suitability of the source to meet the needs of the AGS and gave confidence to designs produced from preliminary estimates.

Because the H ion source and its support hardware form a package which is much larger than the duoplasmatron proton source which it replaces, it had to be located several feet upstream of the entrance to the existing high voltage accelerating column. A low energy beam transport line using a small quadrupole doublet has been designed to match the source output beam to the column. The necessary hardware for this source mounting and beam transport in the Cockcroft-Walton terminal have been built and will be installed in early 1981

A 760 keV beam transport line was designed and components built to take the beam through an achromatic 60° translating section to the existing linac input line. Various schemes for injecting the 200 MeV H^- beam from the linac into the AGS were studied. The design chosen uses a fast collapsing bump to move the circulating proton beam away from the thin carbon foil at which the electrons were stripped from H ions. This approach makes use of existing bump magnets and main ring magnets and eliminates the need for the complex inflecting magnet required for proton injection. Almost all of the remaining injection line components will be retained although some locations will be shifted.

Fast Extraction System

Presently, the FEB line at the AGS provides the primary proton beam for neutrino physics in the North Area. The existing fast extraction system consists of the fast kicker magnets at C15 and D15, a thin septum magnet at E10, and the ejector magnet at H10. The beam presently travels over two betatron wavelengths before final ejection and causes excessive losses and mismatch of the momentum dispersion function. The one microsecond rise time of the C15 kicker usually slices two bunches out of twelve.

The AGS will also be the injector for ISABELLE. The injection scheme uses synchronous bunch transfer from the AGS of twelve bunches to one-fifth of the ISA circumference. The success of injection requires that the AGS fast extraction system deliver twelve clean bunches with little distortion from the kicker.

The new fast extraction system consists of a ferrite fast kicker magnet at H5 and the ejector magnet at H10. The new kicker can rise to its full strength between two AGS bunches and remain sufficiently stable to prevent an increase of the horizontal emittance of the extracted beam. To provide the necessary switching capability, a new pulser system has also been built. It is basically a pulse-forming network discharged into a mismatched load (Fig. 3). The pulse-forming network was shaped empirically to optimize the rise-time and flat-top ripple.

The pulse forming network delivers a 3000 A current pulse to the magnet which settles to the ± 1% flat top ripple within 170 nanoseconds and holds for almost 3 microseconds (Fig. 4). To obtain the fastest possible rise time, the pulse forming network, thyratrons, and other critical components had to be located adjacent to the

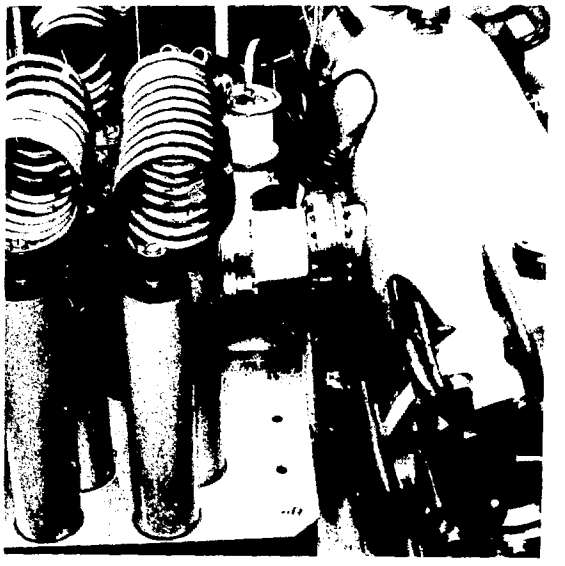


Figure 3. Pulser system for the fast kicker magnet in the new fast extraction system.

magnet in the AGS ring. Tests of the thyratron switch tubes used in the pulser in the AGS ring radiation environment were run over a six-month period resulting in a design which exhibited only 1-2 false triggers per week and no observed deterioration of the equipment.

Other Improvements

In addition to the H⁻ injection work and the H5 ejection kicker development, a number of other AGS systems have had improvements planned, in process, or completed in FY 1980.

The Westinghouse motor-generator (M-G) set used to power the AGS ring magnets prior to acquisition of the Siemens set has been rewound. Work continues to complete the connecting link board hardware and other subsystems which will make the Westinghouse M-G set a back-up for the Siemens.

A prototype system of individual readouts of the ion pump current was installed in the ring to allow better diagnosis of vacuum conditions. Previously these could be read only in groups of ten.

400 W solid state rf amplifiers were installed in the linac to replace the 7651 tube amplifiers in the first stage of the final power amplifier drivers. This should result in less maintenance and downtime.

Work progressed on new computer control interface stations for the Main Control Room. These will utilize touch panels with computer set labels, a color display and a "smart" front end processor.

Neutral Beam Development

The Brookhaven neutral beam development group, which has as its general objective the development of multi-megawatt dc neutral beam systems for fusion devices by the year 1990, shifted its main efforts during this fiscal year from the design of pulsed, non-cooled negative ion sources to the design of cooled steady state negative ion sources. A new idea was tested to make more efficient use of the cathode in magnetron sources by geometrical focusing of H^- ions. This breakthrough, together with optimization of other source parameters, improved the efficiency to 8 kW of source power per ampere of negative ions. These results had a profound effect on the design of the cooled one ampere Mark V dc magnetron, eliminating the difficult nucleated boiling technique and replacing it with simple water cooling. The dc source has been built and its testing has started. In this magnetron source, a hydrogen-cesium plasma is established in an interelectrode gap. The plasma provides the particles to bombard a cesium-coated cathode where negative ions are produced. The ionization efficiency and, therefore, the gas efficiency of such a source is rather low (at best 10%) so that large vacuum pumps are required for a multiampere ion beam. A novel concept is now under investigation to reduce these pumping requirements dramatically by using plasma injection from a tantalum hollow cathode discharge into a magnetron. In a preliminary experiment, the feasibility of this approach has been established when more than one ampere of H^- direct current was produced by the converter. A two ampere steady state negative ion source based on this principle of separate plasma injection from one or more hollow cathode discharges is now under construction.

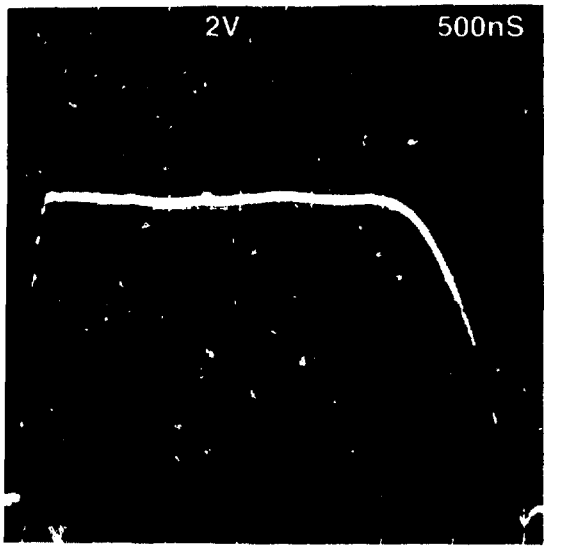


Fig. 4. Output pulse from the pulser system for the new fast extraction system.

Future Plans

Two main projects will continue to occupy the AGS Division in the future. These are preparation of the AGS to be an injector for ISABELLE and the acceleration of polarized protons. The latter will be a joint effort with Argonne National Laboratory, the University of Michigan, Rice University and Yale University.

Planning and Support of the Experimental Program

The Experimental Planning and Support (EP&S) Division is responsible for the operation of the AGS experimental research program. This responsibility includes the development and execution of both long and short range schedules as outlined by the Deputy Director for High Energy Physics. The EP&S staff carries out the setup of radiation shielding and large experimental devices, maintenance and operation of beam separators and cryogenic targets, measurements of magnet characteristics, the installation and maintenance of electrical power and cooling water systems, the maintenance of a large pool of electronics equipment for experiments (HEEP), the safety review of experimental setups, the design of new beams

Beam	Experiment	University
A1	705	BNL/CCNY Vanderbilt Tufts/Mich
A2	Test Beam	Many
A3	735	Yale/BNL
A3	749	Yale/BNL
B1	732	BNL/Ill/Princeton
B1	Test Beam	Many
B2	698	Massachusetts
B4	Test Beam	Many
B4	722	BNL
B5	744	Mass/BNL/Minn/Mich
B6	745	Columbia
C1	726	NYU/BNL
C2	746	BNL/Torino/MIT/Houston/Vassar/CMU
C4	742	BNL/Case Western
C4	723	Wm&Mary/Boston/CMU/CIT/Wyo
C6	708	BNL/Mich St/Syracuse
C8	702	Yale/BNL/Mt. Holyoke
U	737	BNL/Tohoku
U	734	BNL/Brown/KEK/Osaka/Penn/ Stony Brook/Tokyo INS

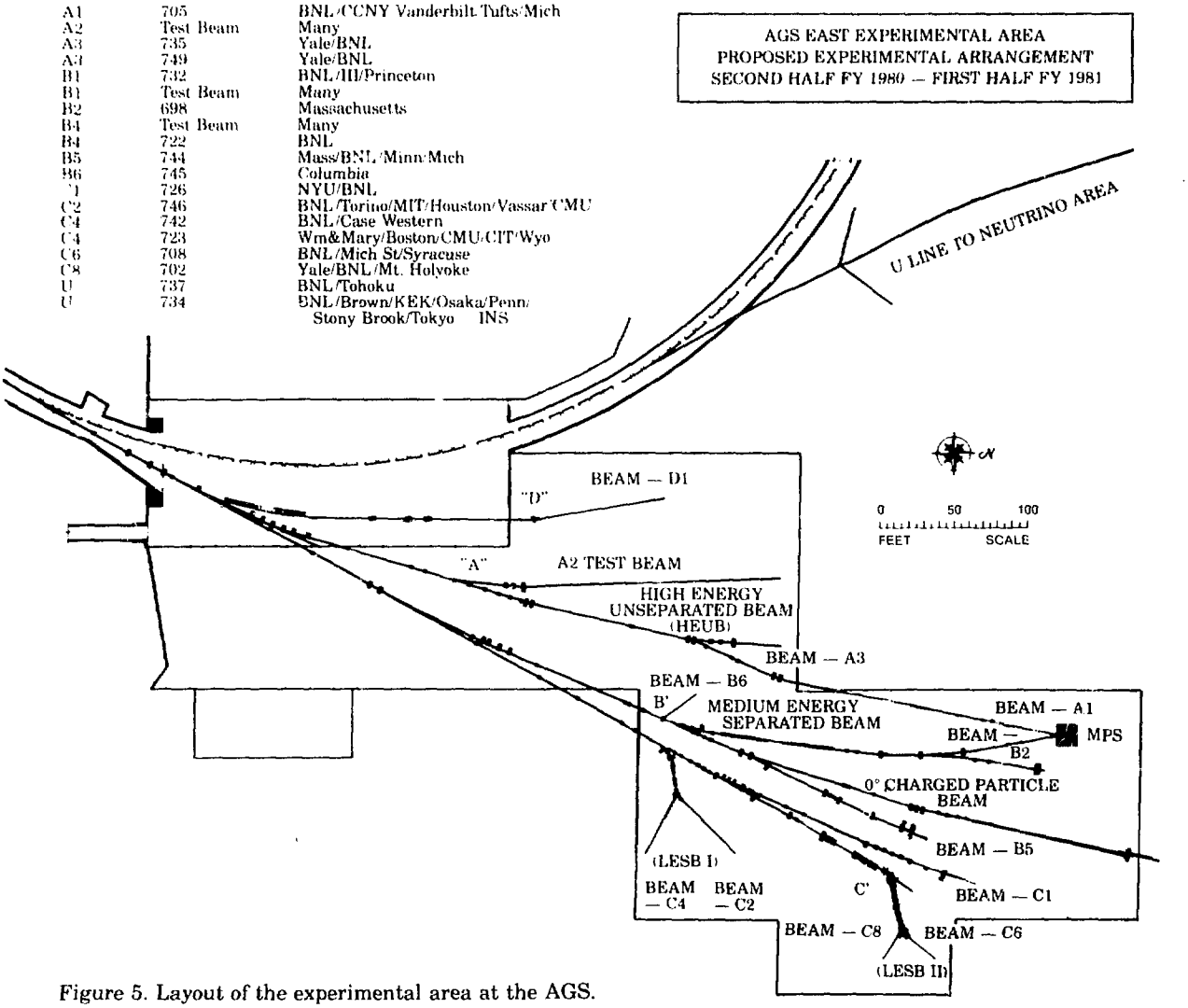


Figure 5. Layout of the experimental area at the AGS.

and experimental facilities, the development of new detectors and electronics, all as required to support the research activities of guest and resident scientist users. Operational crews are maintained on a 24-hour, seven days-a-week basis to operate, service, and provide safety surveillance of the experimental areas and equipment. During FY 1980, the EP&S Division assumed the responsibility for the operation of the On-Line Data Facility (OLDF) and the Multiparticle Spectrometer Facility (MPS).

Eleven experiments were run and 7 were completed in FY 1980 during the 18 weeks of the counter program and the 7½ weeks of the neutrino program. Nine experiments are expected to be run in FY 1981 during the 15 weeks of the counter program and the 10 weeks of the neutrino program. The experimental area layout is illustrated in Fig. 5, and the characteristics of the beams used to support the program are given in Table I. Table II describes both the completed FY 1980 program and the anticipated FY 1981 program.

The major EP&S projects can be classified into three categories: experimental area operations and support; research and development projects; and tasks related to the ISABELLE Project.

Table I

AGS Beam Characteristics

Beam	GeV/c	$\pm \frac{\Delta p}{p}$ (%)	Prod. Angle	Ω (msr)	Flux in thousands/10^{12} protons on target: K^+	K	p	$\bar{p}$	π^+	π^-	@ GeV/c	Purity	Remarks
B4	1.5–6(K) 1.5–9(p)	3	3°	0.3	270	120	2×10^4	300	4×10^4	3×10^4	4	π/K 3	Usually 2×10^{12} ppp; L = 81 m.
C2,C4	≤ 1.1	2	10.5°	2.6	140	80	2×10^4	2	8×10^3	8×10^4	0.75	π/K 10	Usually 2×10^{12} ppp; L = 15 m.
C6,C8	≤ 0.8	2.5	5°	15.0	1000	560	1.4×10^5	14	6×10^5	6×10^5	0.75		Usually 2×10^{12} ppp; L = 15 m.
Separated Beams for Fixed Facilities													
B2	(Same characteristics as B4)												MPS
Unseparated Charged Beams for General Use													
B1	5–24	3	0°	0.3	2500	700	1.5×10^5	200	6×10^4	3×10^4	10		Usually 2×10^{12} ppp; L = 75 m.
C1	5–24	5	0°	0.8	9000	400	3×10^5	30	1×10^5	3×10^4	16	μ/π ≈.03	Usually 2×10^{12} ppp; L = 61 m.
A3	4	12	0°	9.5	8×10^4	4×10^4	2×10^5	6×10^4	1×10^6	8×10^5	4		≤10^{12} ppp + only; alternates with A1; L = 8 m.
Unseparated Charged Beams for Fixed Facilities													
A1	5–24	1.7	0°	0.3	700	17	6×10^5	1.5	1×10^4	3000	18		MPS; L = 130 m; 10^{12} ppp
Neutral Beams for General Use						Λ	K_s	K_l	n				
B5	6–20		4°	0.4		300	27	2×10^4	4×10^5		6–20		10^{10} ppp typical; L = 2.6 m.
Neutral Beam for General Use						ν	$\bar{\nu}$						
U						$10^7/m^2$	$7\times10^6/m^2$					9×10^{12} ppp typical	Fast spill, flux avg. over 0.7 m radius, peaks at 1.5 GeV/c.

Table II

Experimental Programs, completed or in progress in FY 1980 and anticipated in FY 1981.

Beam	Exp. No.	Institution Description of Experiment	
A1	705	BNL/CCNY/Vanderbilt/Tufts/Michigan State Search for narrow and broad resonances from π^-p interactions. The double V states in π^- p → $\Lambda\bar{\Lambda}/K^0_s K^0_s/\Lambda K^0_s$ + neutrals are studied for resonant structure. (MPS).	Completed.
A3	735	Yale/BNL Observation of transverse μ polarization in this decay would be evidence for a time-reversal invariance violation. The π's will be identified by detecting the γ rays from their decays in a lead glass array, and the muons will be analyzed in a magnetic spectrometer and stopped in aluminum plates. The muon polarization will be measured by precessing the magnetic moment in a weak field and observing the decay electron.	To be completed.
B2	698	U. Mass Polarized target physics with the MPS. A "spin refrigeration" polarized target has been built which requires neither microwave nor a highly uniform magnetic field. It has been installed in the MPS. $K^-p\uparrow \rightarrow Y^*\pi \rightarrow \Lambda\pi^+\pi$ reactions are studied near 2 GeV/c.	Completed.
B5	744	Mass/BNL/Minnesota/Michigan Measurement of inclusive Σ° production and polarization. Σ° produced in p + Be → Σ° + X are analyzed by the decay $\Sigma^\circ \rightarrow \Lambda\gamma$ $\Lambda \rightarrow p\pi^-$ The γ's are detected in a lead glass array and parity-violating Λ decay is analyzed for polarization in a magnetic spectrometer.	Completed
C1	726	New York University/BNL Search for charm in hadronic interactions near threshold. The reactions: 1. $\pi^+p \rightarrow D^0C_1^{++}$ $C_1^{++} \rightarrow K^+K^+$ 2. $\pi^-p \rightarrow D^0D^-p$ $D^- \rightarrow K^-\pi^+$ 3. $p\bar{p} \rightarrow D^0D^0$ $D^0 \rightarrow K^-K^+$ will be studied. The final two decay particles will be analyzed in a large aperture spectrometer, with sensitivity estimated to be better than 20 nb.	To be completed.
C1	732	BNL/Princeton/Illinois Search for the η_c. The reaction $\pi^-p \rightarrow \eta_c n$ $\eta_c \rightarrow \gamma\gamma$ is studied. The γs are detected in a lead glass array, and the neutron time-of-flight measured.	Completed.

Table II (cont'd)
Experimental Programs, completed or in progress in FY 1980 and anticipated in FY 1981.

Beam	Exp. No.	Institution Description of Experiment	
C2	746	BNL/Torino/MIT/Houston/Vassar/CMU Spin and isospin effects in light hypernuclei. The hypernuclear spectrometer is used to investigate $^{A}Z(K^-,\pi^-)^{A}_{\Lambda}Z$ with $\theta_{K\pi} = 0°$ for $^{10}_{\Lambda}B$, $^{13}_{\Lambda}C$, $^{14}_{\Lambda}N$, and $^{15}_{\Lambda}O$.	Completed.
C2	752	Houston/BNL/CMU/Vassar A search for hypernuclear levels in ^{16}O in the (K^-,π^+) reaction The hypernuclear spectrometer is used to investigate $^{A}Z(K^-,\pi^+)^{A}_{\Lambda}Z$ with $0° \leq \theta_{K\pi} \leq 15°$ for ^{16}O.	To be completed.
C2	760	MIT/BNL/Torino/Houston/NYU/Vassar/Peking Spin dependence of the Lambda Nucleus interaction determined by observation of hypernuclear gamma rays. The hypernuclei to be studied are $^{7}_{\Lambda}Li$, $^{9}_{\Lambda}Be$, and $^{16}_{\Lambda}O$.	To continue.
C2	742	BNL/Case Western Reserve Search for the S meson in the total and elastic $\bar{p}p$ cross section. These cross sections are measured using a relatively "massless" proportional chamber which should resolve the controversy surrounding the S(1936) meson.	To be completed.
C6	708	BNL/Michigan State/Syracuse/DOE Search for γ transitions in $\bar{p}p$ annihilations at rest and low energies. γ rays coincident with antiproton annihilations in H_2 are to be converted in a lead sheet and the momentum of the resulting e^+e^- pair analyzed in a pair spectrometer yielding a very precise measurement of the γ energy with excellent resolution.	To be completed.
C8	702	Yale/BNL/Mt. Holyoke Measurement of the asymmetry in the radiative decay $\Sigma^+ \rightarrow p\,\gamma$ from polarized Σ^+ hyperons. Polarized Σ^+ hyperons are produced forward in the reaction $K^-p\uparrow \rightarrow \Sigma^+\uparrow\pi^-$ on longitudinally polarized protons using the backward π^- as a trigger. The Σ^+ decay is selected on the basis of time-of-flight in a spectrometer and the decay proton kinematics.	To be completed.
U	704	Harvard/BNL Search for oscillations of a long-lived neutrino beam. The time evolution of a long lived ν_μ beam is studied searching for a ν_e signal in a large detector. Primary 1.5 GeV/c protons are used to produce a high-flux, low background beam.	Completed.
U	734	BNL/Brown/KEK/Osaka/Penn/Stony Brook/Tokyo-INS Measurement of elastic scattering of neutrinos from electrons and protons. These are weak neutral-current processes. The outgoing electron or proton in the reactions $\nu e \rightarrow \nu e$ $\nu p \rightarrow \nu p$ will be identified by their characteristic behavior in a large scintillator-proportional drift tube detector.	To continue.
U	737	BNL/Tohoku Study of neutrino interactions in deuterium in the 7-ft Bubble Chamber.	Completed.

EXPERIMENTAL AREA OPERATIONS AND SUPPORT

The new switchyard for the slowly extracted beam was installed and commissioned. The combined proton extraction and transport efficiency rose from 60% to over 90%. Construction began on the proton transport to the fourth primary target station, called the D target. This project includes new 6 tesla superconducting dipoles. It is anticipated that the D line construction will be completed in FY 1982. Figure 6 shows the electrostatic septa which divide the beam into four branches.

Three secondary beams were either rebuilt or modified. The B4 medium energy separated beam (MESB) was modified for the ISABELLE test beam facility. Both MESB separators were rebuilt for more reliable high field operation. A high energy unseparated beam, C1, was rebuilt and commissioned to incorporate a high resolution momentum tagging spectrometer for an NYU/BNL charm search. The neutral beam, A3, was rebuilt and commissioned into a K^+ beam for a Yale/BNL experiment to test time reversal invariance.

The movement of shielding, 12,600 tons (m) of concrete and iron, a 2500 ton (m) cyclotron magnet and coils and an assortment of magnets and power supplies from the Space Radiation Effects Laboratory (SREL) was completed. The installation of the neutrino-electron and neutrino-proton elastic scattering experiment blockhouse was completed with the shielding obtained from SREL. The blockhouse is 36.6m long and 18.3m wide. The SREL stopping muon channel will be used to build a stopping muon beam for a Columbia/CERN QED experiment and a Bell/BNL/Wm&Mary/George Mason University/Virginia State University material sciences experiment on muon spin rotation. The preparation and modification of components was begun in FY 1980. This work is being done at Nevis Laboratory.

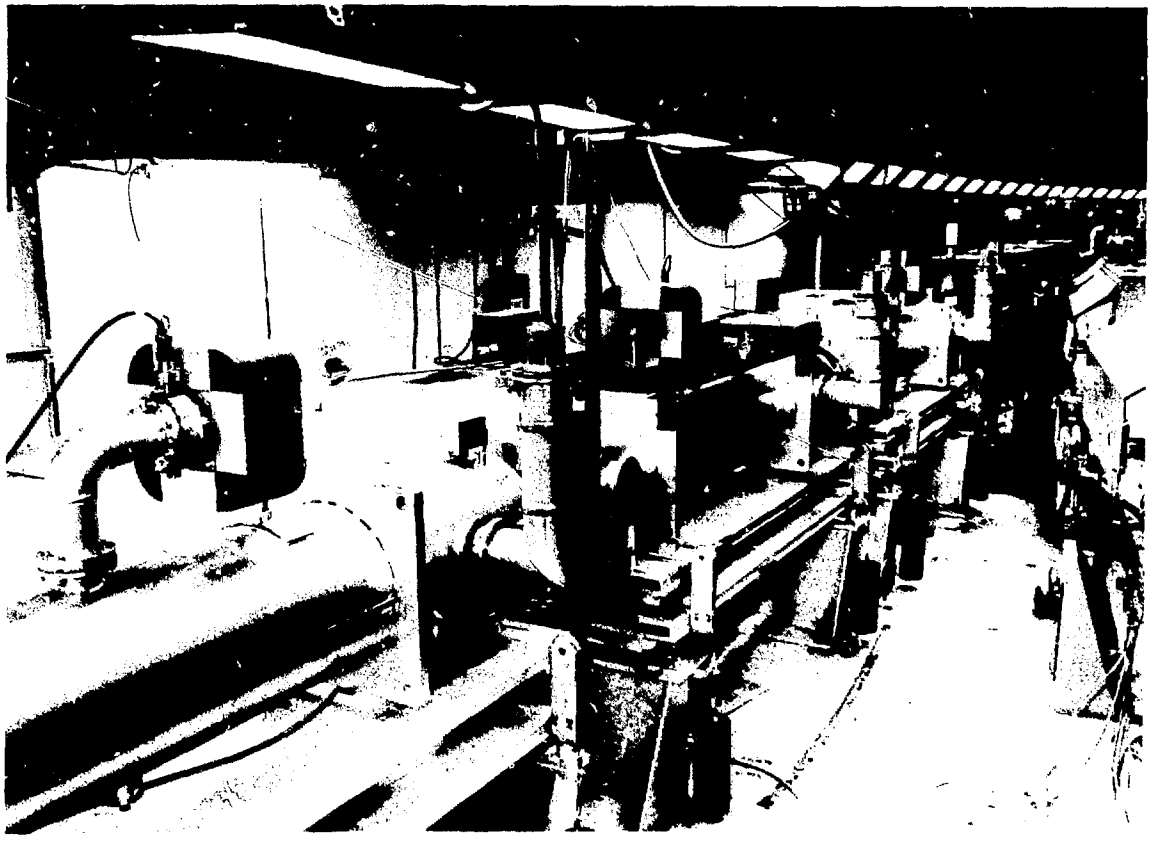


Figure 6. Electrostatic septa which divide the primary proton beam.

Prior to the startup of the experimental program at the MPS, the power supply for the MPS magnet (a series-parallel setup of four 600 kW power supplies) was replaced by the unit which was previously used to power the 80-inch bubble chamber magnet. Significantly more reliable performance was obtained from the new setup.

SUPERCONDUCTING POWER CABLES

The major project is the development and demonstration of very high power underground transmission using superconducting cables. A cable taping "factory" has been constructed to manufacture short lengths of the flexible cable under development. About 45m of trial cable was made with the full insulation thickness for 138 kV operation. The cable was used for assessment of fabrication techniques, bend performance, and high voltage evaluation. A cable termination rated for 4000 A, 60 Hz, and 138 kV operation has been designed and tested in the laboratory. A test facility for full power testing has been constructed and the cable enclosure has been cooled to the correct operating temperature. All the power supplies for testing two cables to the 4000 A, 138 kV level have been installed and tested in the past year.

Another project is the development of a highly oriented polymeric insulation for very high voltage transmission cables of a more conventional type. Electrical testing of the new insulation has started and a 91.4m test loop was designed and is now out on bid.

RESEARCH AND DEVELOPMENT

A program of beam instrumentation improvements was initiated in conjunction with the reconstruction of the switchyard. New designs for position and profile monitors, segmented wire ionization chambers, and intensity measuring secondary emission chambers were completed. Their performance is under evaluation. Of importance is their susceptibility to radiation damage by the higher intensity proton beams available with the new switchyard.

The ongoing electrostatic separator effort has now been able to shape the fields and reduce the field gradients so that the operation of separators at greater than 800 kV is possible.

In the detector areas, the MPS group has been developing a set of three fine cell drift chambers. Two modules were successfully tested this year in the MPS as part of the preconditions to approval of upgrading the rest of the MPS. In conjunction with both BNL and MIT, an extensive program of investigation of the physical and practical limits of track resolution for precise momentum measurement in drift chambers has begun. This study also includes the study of effects of systematic errors on the ultimate accuracy of track measurement in large multilayer drift chambers. A first cell of a 4.5m long , 2m outside diameter, 100 wire cylindrical drift chamber has been constructed.

In the electronics area, the MPS group will continue to study the performance characteristics of three integrated circuits (amplifiers, discriminators, and digital delay-shift registers) which are being custom developed by industry. The amplifier and discriminator circuits have met specifications and are under construction. The digital delay-shift register is in the final pre-production phase. These chips will be used in the new drift chamber readout. Both the MPS group and high energy equipment pool group (HEEP) are participating in the development of FASTBUS, a modular system which integrates the data acquisition electronics with the online computer. The MPS group has developed a conceptual design for the upgraded MPS, while the HEEP group has assisted Experiment 735 (Yale/BNL) with the design and production of FASTBUS modules, crates, segment interconnects, etc. The Yale/BNL group successfully

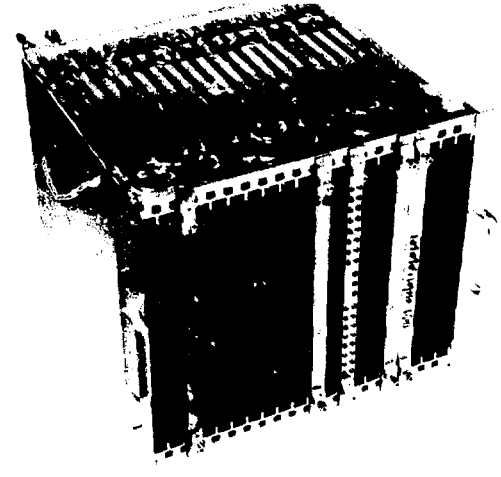


Figure 7. Conduction-cooled FASTBUS crate with a few modules installed.

used this new system in an AGS experiment. Figure 7 shows a FASTBUS crate with a few modules.

TASKS RELATED TO THE ISABELLE PROJECT

The support of an ISABELLE alternate magnet effort, a test beam facility, and the developments in drift chamber detectors, integrated circuits, and FASTBUS are directed to the future. In addition to these items, the EP&S Division is actively involved in several aspects of the ISABELLE project through its participation in a number of task forces. Design of the proton beam transfer lines from the AGS to ISABELLE and the development of a facility for testing the effects of radiation heating on ISABELLE superconducting dipoles are two such efforts. The work on superconducting dipoles for the proton transport to the U target station and the new D target station now forms the basis of a design for ISABELLE ring magnets that will provide an alternative to the "cos θ" design described in the later section on the ISABELLE project, which is to provide a backup in case the cos θ design should prove to be unacceptable. Conceptual design work has begun on a joint effort to construct large superconducting coils such as might be used for a large dipole or solenoid experimental magnet. Conceptual work has begun on 7.5-10 tesla dipole compensating magnets for the ISABELLE crossing regions.

ACCELERATOR DEPARTMENT

J.R. Sanford — Chairman

L.W. Smith — Deputy Chairman

J.J. Grisoli
D. Lazarus **Assoc. Chairmen**

J.E. Becker — Business Office

AGS DIVISION
Y.Y. Lee — Head

EXPERIMENTAL PLANNING & SUPPORT DIVISION
D. Lowenstein — Head

ATA DIVISION
E B. Forsyth — Head

AGS DIVISION

Y.Y. Lee — Division Head

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H Ion Source Development and Accelerator Physics Research

L. Ahrens
Accelerator Physics, Low Field Corrections, Instability and RF Pick-Up Electrodes, Polarized Protons, Physics Research

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Chief AGS Operations, H Injection Physics Research

D.A. Davis
Deputy Division Head, Power Distribution

D. Edwards, Jr.
AGS and ISA Transfer, Vacuum System Physics Research

G. Gammel
Heavy Ion Fusion Project, Low Beta Acceleration, Physics Research, MEQALAC Development

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H Ion Source Development, Physics Research

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AGS Division Head, Fast Extraction System, ISA Transfer, Polarized Protons, Physics Research

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Heavy Ion Fusion Project, MEQALAC Development, Physics Research

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Mechanical Engineering, H Ion Source Project

R. Mobley
Preaccelerator Developments, Physics Research

K. Prelec
H Ion Source Development, Physics Research

Th. Sluyters
H Source and Acceleration, Physics Research

H. Weisberg
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W.T. Weng
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Alan S. Carroll
Beam Design, Experimental Area Liaison, Particle Physics Research, Superconducting Magnet Development

I-Hung Chiang
Detectors, Electronics, Experimental Area Liaison, Particle Physics Research

Gordon T. Danby
ISA Superconducting Magnet Properties, Superconducting Magnet Development

Basil DeVito
Mechanical Engineering, Superconducting Magnet Development

Asher Etkin
Experimental Area Liaison, Multiparticle Spectrometer Facility, Particle Physics Research, Scheduling Physicist

Derek I. Lowenstein
Control Systems, Division Head, ISA Detector Magnets, Particle Physics Research

Yousef Makdisi
Experimental Area Liaison, ISA Superconducting Magnet Properties, Particle Physics Research

Thomas W. Morris
Multiparticle Spectrometer Facility, Particle Physics Research

Albert G. Prodell
Cryogenics, ISA Superconducting Magnet Properties

Alfred C. Saulys
Multiparticle Spectrometer Facility, Particle Physics Research

S. Peter Yamin
Beam Design, Detectors, Experimental Area Liaison, ISA Magnet Development Particle Physics Research

ATA DIVISION

E.B. Forsyth — Division Head

A. Ernst
Cable Insulation Development and Technical Monitoring of DOE Contracts.

R.J. Gibbs
Cryogenic Engineering of the Test Facility.

W.E. Harrison
Control and Instrumentation Engineering. Also Administrative and Budget Control Responsibilities.

J.E. Jensen
Deputy Manager of Superconducting Power Transmission Development. Coordination of Cryogenic and Mechanical Engineering.

C.J. Klamut (Part-time DEE)
Fabrication of Superconducting Tape.

T.R. Muller
Construction and Operation of the Taping Machine.

A.J. McNerney
High-Voltage Testing of Cable Insulation and Terminations.

K.F. Minati
Mechanical Engineering of Laboratory Equipment and Terminations.

G.H. Morgan
Deputy Manager of Superconducting Power Transmission Development. Coordination of Scientific Effort.

A.C. Muller (DEE)
Development of Polymeric Insulation for Both Superconducting and Room-Temperature Cables.

R.A. Thomas
Low Temperature Physics and Instrumentation.

F. Schauer (Visiting Appointment)
Design of High Voltage Bushing and Analysis of Power Losses of Superconducting Cables.

I. Ishii (Visiting Appointment)
Low Temperature Dielectric Insulation Development

The ISABELLE Project

In 1978 construction at Brookhaven National Laboratory of a proton-proton colliding beam facility was started. This facility, known as ISABELLE, will be one of the most powerful instruments available worldwide in the 1980's to carry out particle physics research. It will consist of two identical magnet rings for the accumulation, acceleration, and storage of protons. The two rings are in the same horizontal plane allowing for intersections at six crossing points where the counter-rotating beams collide with each other. The outstanding features of ISABELLE will be the high center-of-mass energy available from the head-on collisions. With 400 GeV in each beam, the available energy is equal to that from a 340 TeV beam striking a stationary target.

Many experiments are possible due to ISABELLE's broad operating range covering the energies from injection at 30 GeV to peak field at about 400 GeV. ISABELLE will provide a high luminosity compared with the antiproton-proton colliding beam experiments now under construction at CERN and FNAL. The luminosity at ISABELLE is projected to be 2×10^{32} $cm^{-2}sec^{-1}$ in the standard insertions at top energy. Modifications to the insertion layout should eventually allow luminosities of about 10^{33} $cm^{-2}sec^{-1}$. These luminosity levels can be achieved with 8 A beams in each ring. The expected interaction rate reaches about 40 million per second resulting in a total particle production rate at top energy on the order of 1 billion per second at each crossing.

Figure 1 shows the layout of ISABELLE on the Brookhaven site and Table I, some important machine parameters. A circular tunnel, 4¾ times that of the AGS in circumference, will contain the two adjacent magnet rings consisting of superconducting dipoles and quadrupoles. Successive pulses of protons from the AGS will be injected at 29.4 GeV into both rings, captured and debunched. When a circulating current of about 8 A is accumulated, the stacked beams will be rebunched and accelerated to full energy in approximately 8 minutes.

The long acceleration cycle and the storage operating conditions at ISABELLE suggested the use of superconducting magnets. This results in a reduction of electric power consumption and a considerably reduced tunnel circumference. Construction of superconducting magnets requires a new technology, which unfortunately, is turning out to be more arduous than had been anticipated, and a number of full-size preproduction dipoles performed below expectation. Substantial efforts have been mobilized during 1980 to develop an adequate understanding of the dipole limitations and to improve the performance of the ISABELLE magnets. A number of improved R&D magnets have been built and tested. Great progress has been made in understanding these magnets and the performance of the improved models is most encouraging with the design field of 50 kG being reached, albeit after many training quenches.

Conventional construction is proceeding with completion expected in April 1983. A major intermediate milestone will be the cooldown

Table I

Abridged Table of ISABELLE Parameters

Energy	
Maximum energy	~400 + 400 GeV
Equivalent accelerator	340 TeV
Magnet System	
Circumference (4¾ x AGS)	3834 m
Bending field for 400 GeV	50 kG
Total number of dipoles	732
Total number of quadrupoles	352
Vacuum chamber diameter	8.8 cm
Injection	
AGS energy	29.4 GeV
ISA current/ring	8 A
Number of protons/ring	6.3×10^{14}
Acceleration	
Duration	8 min
Energy gain/turn	11 keV
Peak rf voltage	36 kV
Experimental Regions	
Number	6

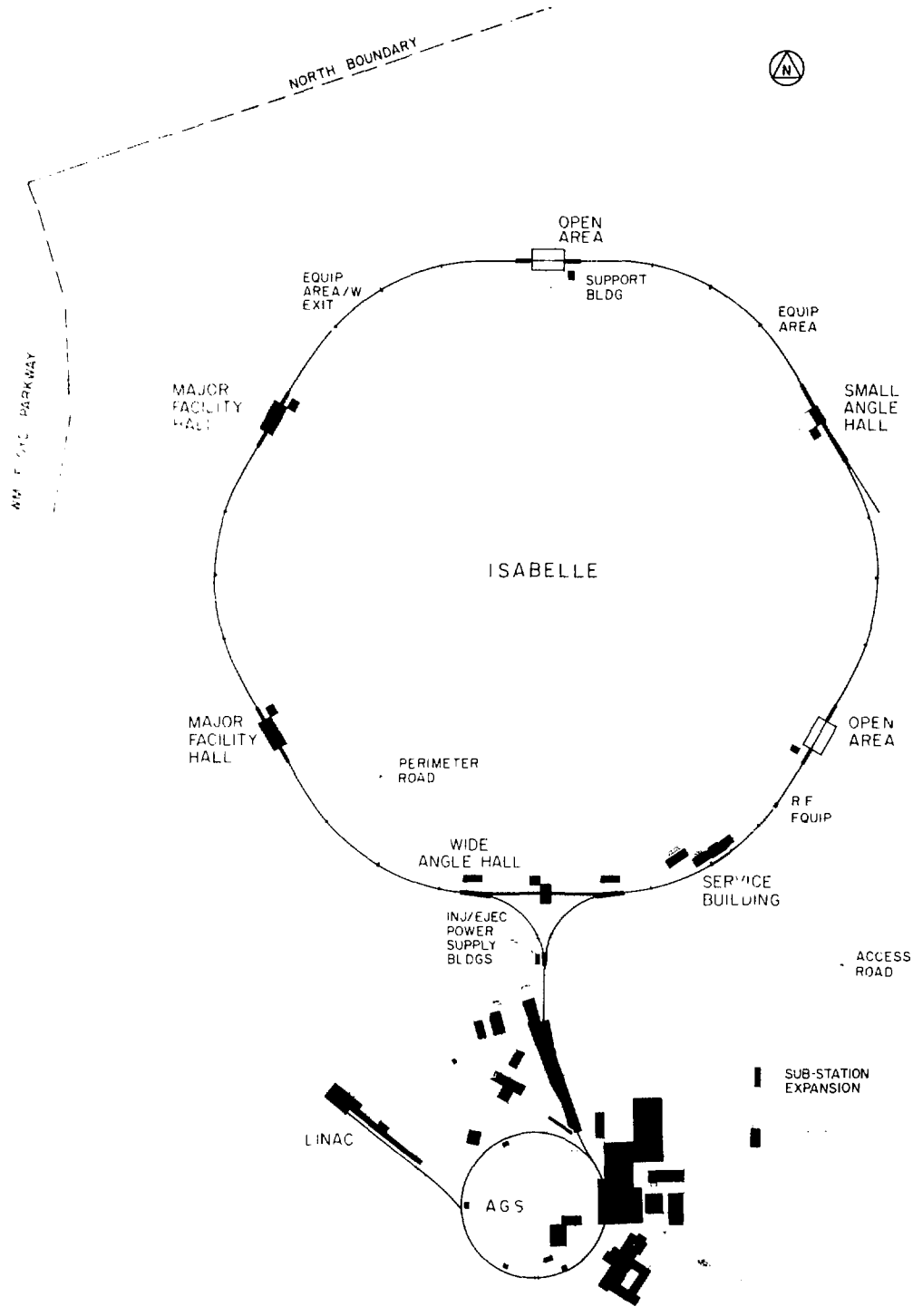

Figure 1. Layout of ISABELLE facility in the northwest corner of the Brookhaven site, showing its relation to the existing AGS.

and testing of one sextant scheduled for early in 1984. Overall completion of the ISABELLE project would then occur in 1987.

CONVENTIONAL CONSTRUCTION

Conventional facility construction was initiated by ground breaking ceremonies in October of 1978 and actual site clearing in January of 1979. Since the start of actual magnet enclosure construction, considerable progress has been made in 1980 on the construction of magnet enclosure and certain experimental areas. The entire magnet enclosure is now erected with the exception of the Injection/Ejection section of the machine. Approximately 10% of the earth embankment remains to be done over the magnet enclosure. In addition, the remaining topsoil and seeding will be accomplished in the spring of 1981. Figure 2 shows the interior of the magnet enclosure.

As indicated in Fig. 1, there will be four experimental halls and two open areas where experiments can be installed in temporary structures. Construction has progressed so that the Wide Angle Hall at six o'clock is about 75% complete, and the Narrow Angle Hall at two o'clock is about 10% complete. The Wide Angle Hall is shown in Fig. 3. The Compressor Building and Cryogenic Wing of the Service Building is under contract and about 10% complete. In addition, work on the Injection/Ejection Beam Tunnel has been started. The existing 69kV Substation Switchyard and building has been enlarged and electrical switchgear is being installed. This work is over 60% complete.

Designs for the Service Building, Major Facility at ten o'clock, and the twelve o'clock areas were partially completed in 1980. Utility designs were initiated in 1980 and are 50% complete.

SUPERCONDUCTING MAGNETS

The long acceleration cycle and the storage operating conditions at ISABELLE motivate the use of superconducting magnets. Not only is power consumption reduced, but very high

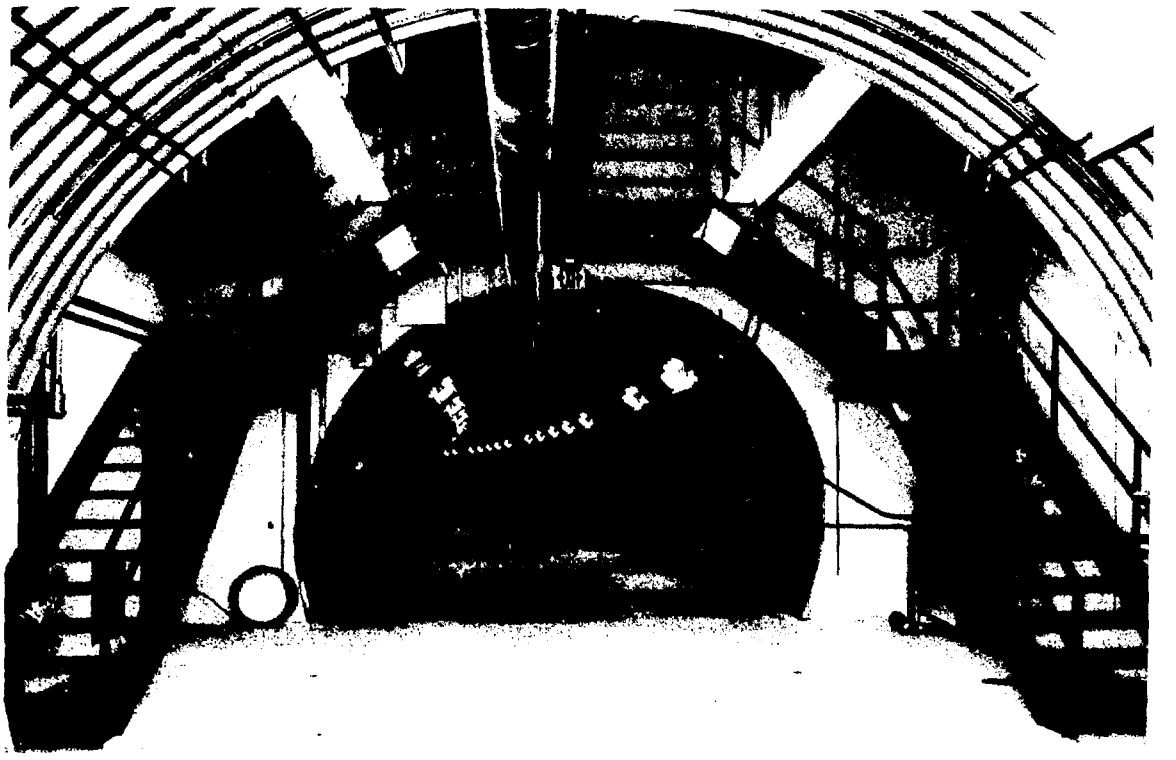

Figure 2. Interior of the magnet enclosure seen from one of the equipment areas. The two magnet rings will be installed in this enclosure.

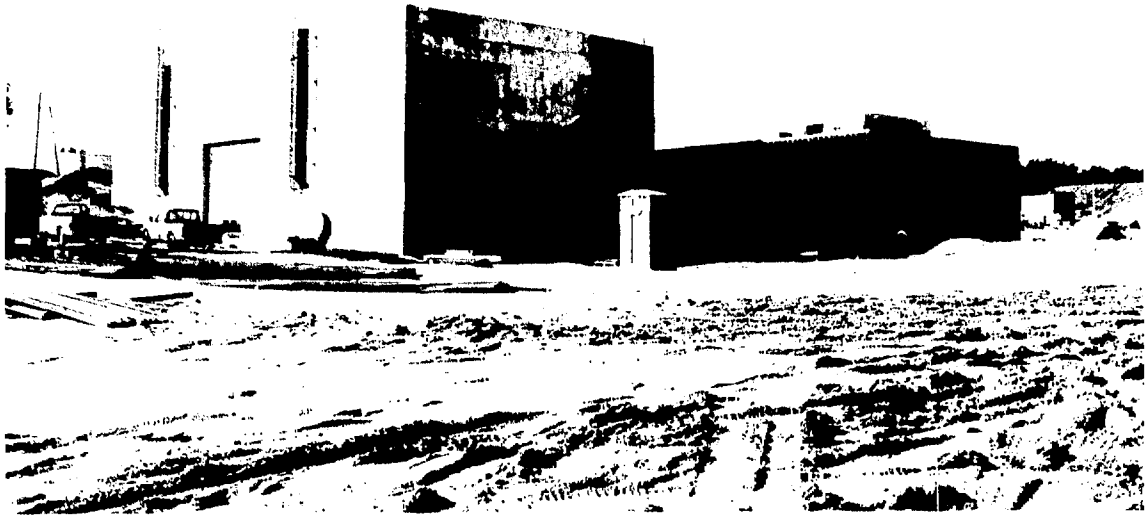

Figure 3. Wide Angle Hall.

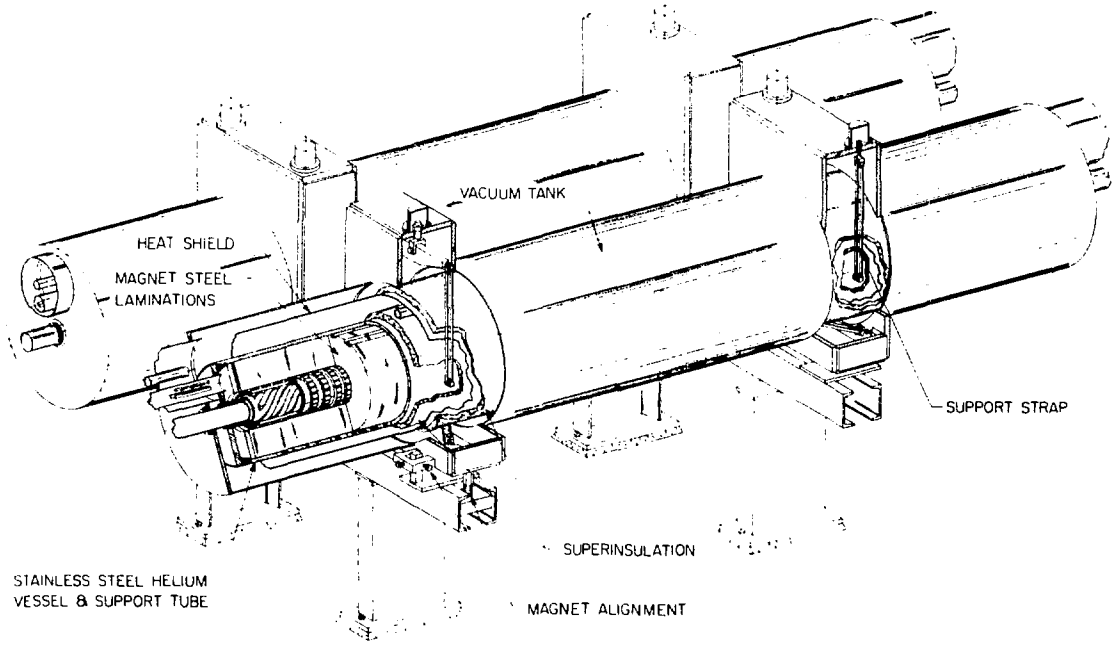

Figure 4. A pair of ISABELLE dipole magnets with supporting structures and insulating vacuum tanks as they will appear in the magnet enclosure.

magnetic fields are feasible with this approach. There are 732 dipole and 352 quadrupole magnets, approximately 5 m and 2.5 m long respectively, in the ISABELLE lattice. They are wound from a braided multifilamentary NbTi conductor. The long "saddle coils" are fabricated by a high pressure molding technique and clamped firmly on an underlying cylindrical bore tube by a stack of iron laminations, which provides a return path for the magnetic flux and provides mechanical constraint against the forces generated at the magnetic field of 50,000 G and the operating current of 4,000 A. The magnets are cooled by forced circulation of super-critical helium at 3.8K and five atmospheres pressure. Figure 4 shows an isometric view of a pair of assembled dipole magnets in their cryostats.

In the fall of 1979, the second batch of the preproduction prototype dipole magnets wound at Westinghouse (altogether involving twelve dipoles and two quadrupoles) were tested. A shortcoming experienced with the initial batch of these dipoles which resulted in coil damage due to excessively slow propagation of the resistive zone when the magnet reverts to the non-superconducting state during a "quench" had been overcome. However, there remained the serious problem of the magnets requiring an unacceptable number of "training" quench steps to reach the full operating field of 50 kG.

Consequently, a major effort was launched in the winter to obtain basic analytical insight into the causes of the training problem—diagnosed as due to conductor motion from the rapidly building electromagnetic forces at high fields. This motion causes premature de-excitation from heat produced by the resulting friction. The conclusions of this analysis were applied to a new series of dipoles constructed in-house at a much accelerated pace. The main features of these magnets are a) improved coil rigidity, b) firmer coil support, and c) provisions for slip planes within the coil structure to minimize effects of friction.

The first of the new series of magnets, MK 17, was completed in late spring of the year and the first clear success of these efforts came in September when MK 18 reached the design field in a modest number of training steps as shown in Fig. 5. As the reporting period closed, approximately a dozen further dipoles, and several new quadrupoles, incorporating certain other important construction features in addition to the aforesaid modifications, were in various stages of preparation.

The new program has been augmented by an R&D Group within the Magnet Division for undertaking laboratory-scale investigations of the electrical and mechanical sub-components. A facility is now available for testing modest size coil windings subject to the fields and forces prevailing in an actual magnet. By this coil simulation technique one can investigate such parameters as quench front propagation velocity, energy necessary to trigger a quench, critical current in the superconductor, coil porosity, etc., under realistic yet controlled conditions.

ACCELERATOR COMPONENTS

A storage ring facility such as ISABELLE requires a detailed study of many aspects of beam dynamics to assure that the design is consistent with the performance goals. The machine lattice, i.e., the actual arrangement of the

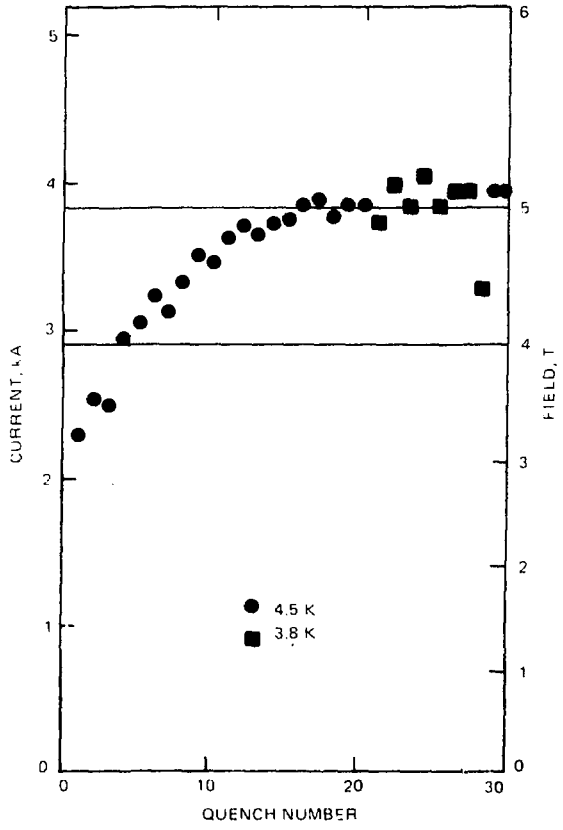

Figure 5. Quench curve, i.e., excitation level versus number of training steps, for dipole MK 18.

bending and focusing magnets, has now been completely specified and the position coordinates of the magnets have been translated into the actual numbers to be used by the survey crew. With this design complete, the actual construction of components can proceed.

The largest single item is the refrigeration system. This system is logically divided into three parts, the compressor system, the distribution system, and the cold box consisting of heat exchangers and turbo-machinery. The cold box has been ordered, the vendor has finished detailed design, and fabrication has begun. The first vacuum tank for the cold box is shown in Fig. 6. At BNL, design work continued on the compressor system and the distribution system. Many of the concepts of this refrigeration system have been studied in the "First Cell".

The "First Cell" is a group of four developmental magnets which have been assembled into a system resembling a small portion of ISABELLE. The assembly was done in a mock tunnel section and techniques were developed for handling the magnets in this cramped environment and for making the electrical, cryogenic, and vacuum connections between them. The system was connected to the "R&D" refrigerator through long transfer lines designed to simulate some of the cryogenic lines to be used in ISABELLE. A view from the open end of the mock tunnel section is shown in Fig. 7.

Cryogenic tests have revealed several fabrication problems, most of which have been corrected. The information obtained will be used to avoid such problems in ISABELLE itself. The magnet string has now been cooled to about 4.6 K and electrically powered to low levels for tests of power supplies, interlocks, and the wiring system. Further testing of this system will provide information on the insulating vacuum system and the ultra-high vacuum system for the beam.

Work has been proceeding on many other components of the accelerator. Power supplies for the magnets and the correction coils are designed, and some of the final units are fabricated and in use in the magnet test program. The rf cavities have been designed, models have operated to full capacity, and a scheme has been developed to keep their impedance low enough to avoid beam instabilities. Considerable progress has been made on the power amplifier design required for the cavities. The computer

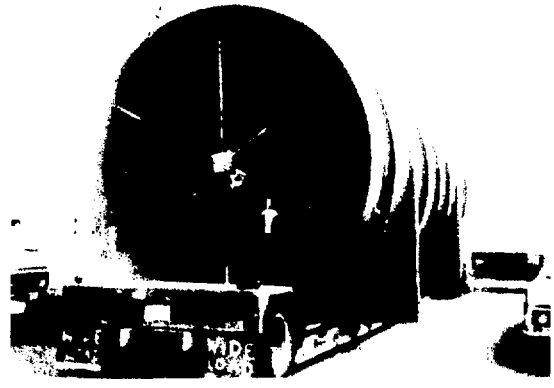

Figure 6. Vacuum tank #1 of the ISABELLE refrigerator cold box at the Helix Process plant.

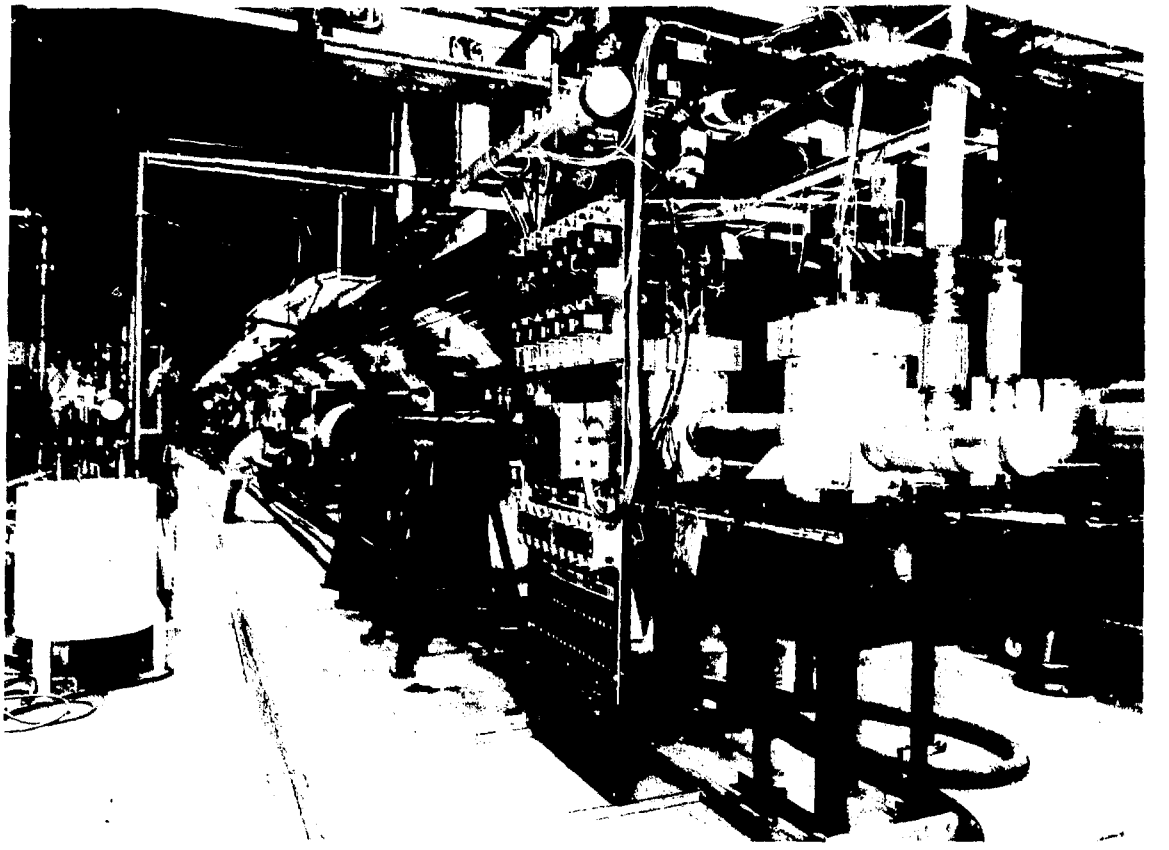

Figure 7. The "First Cell" test system showing magnets, transfer lines, and other components in the mock tunnel section.

control system design has also progressed. A complete system for propagating data between the control room computers and the various hardware devices in the accelerator has been developed. Also a language to be used for communicating with operators and users has been specified. The injection line hardware has been designed. Magnets for the two 90° bends are being fabricated and models for the kicker and system magnets are under test. All aspects of the high vacuum system are designed and prototypes have been tested. The tests have included a computer controlled bake-out cycle for a complete cell of eight units.

ISABELLE PROJECT

J.R. Sanford Project Head
K. Johnsen Deputy Project Head

H. Hahn	Assistant Project Head	D.H. White	Head, Experimental Facilities Div.
J. Spiro	Assistant Project Head		
M.Q. Barton	Head, Accelerator Div.	R.W. Young	Safety Officer
R.I. Louttit	Deputy Div. Head	F. Thornhill	Safety
E.J. Bleser	Head, Magnet Construction Div.	M. Shear	Quality Assurance Officer
		V. Gutierrez	Quality Assurance
H. McChesney, Jr.	Head, Administrative Div.	W. Morrison	Quality Assurance
		E.W. Dexter	Administrative Engineer
E.P. Rohrer	Head, Construction Div.		

ACCELERATOR DIVISION

This Division is responsible for the design and construction of all accelerator systems, except the superconducting magnets. They also have responsibility for the installation of all systems into the magnet enclosure.

Theory: Analytical studies, numerical calculations and computer simulations of particle beam dynamics and the behavior of accelerator components.

M. Cornacchia	C. Goodzeit	C. Pellegrini
E. Courant	K. Jellett	J. Poole
G. Dell	M. Month (on leave)	R. Ruth (part-time)
J. Donhowe	G. Parzen	J. Wang

Injection/Ejection: Design and construction of beam transport system from AGS into ISABELLE rings, proton beam ejection system and beam dumps.

H. Foelsche	A. Kaam	R. Nawrocky
J. Baron	J. Keohane	C. Schmidt
J. Claus	P. Montemurro	R. Thern
S. Ghoshroy		J. Tuozzolo
D. Gough		P. Zuhoski

Electrical Components: Design and construction of magnet power supplies, rf power supplies, controls, computer systems and monitoring equipment.

J. Humphrey	S. Giordano	M. Plotkin
D. Brownstein	A. Herman	M. Puglisi
W. Buxton	K. Hillman	E. Raka
R. Edwards	S. Kennell	M. Shapiro
E. Ezura	B. Morris	E. Tiagha
R. Frankel		F. Tinta
G. Ganetis		R. Warkentien

Cryogenics: Helium refrigerators for development work and for ISABELLE, helium distribution and special low temperature devices.

D. Brown	Y. Farah	W. Schneider
M. Afrashteh	A. Fresco	J. Sondericker
J. Bamberger	A. Schlafke	K. Wu

Vacuum: Vacuum vessels, pumps, measuring devices and leak-checking procedures.

H. Halama	J. Dovydaitis	H. Hseuh
T. Chou	C. Foerster	P. Stattel

Installation: Survey, precision location and installation of components in magnet enclosure.

I. Polk	J. Cottingham	S. Plate
F. Atkinson		R. Rosenka
S. Baker		M. Woodle

MAGNET DIVISION

This Division is responsible for the design and construction of all superconducting magnets.

Coil Production: Winding superconducting coils and assembling complete dipole and quadrupole magnets.

L. Repeta	R. Kehl	R. Oram
A. Bertsche	R. LeRoy	G. Tanguay
V. Buchanan	S. Mai	C Theisen
J. Cullen	W. McGahern	P. Thompson
E. Grove	R. Occhiuzzo	W. Velia
R. Hodor		W. Zeman

Development: Improvements to superconducting braid and other materials, with measurements on short samples and simulated coils.

W. Sampson	J. Kaugerts
C. Holbrow	S. Moehlecke

Planning & Analysis: Coordination of development, tests, and production and the analysis of results.

M. Tannenbaum	A. Greene	G. Reiter
P. Dahl		P. Wanderer

Testing & Measuring: Powering magnets at operating temperature, current, and ramp rate, with precision measurement of magnetic field properties.

R. Engelmann	K. Jaeger	C. Sylvester
G. Bozoki	H. Kirk	M. Thomas
D. Gardner	J. Koehler	A. Wijancgo
J. Herrera	K. Robins	E. Willen

EXPERIMENTAL FACILITIES DIVISION

This Division is responsible for the design of ISABELLE experimental areas, the design and construction of detectors, and development of systems for data acquisition.

Experimental Areas: Evaluation of overall requirements for the future experimental program and design of experimental area buildings.

S. Aronson
B. Gibbard
P. Gollon (part-time)
E. Siskind
A. Stevens
A. Thorndike
W. Walker

Detector Development: Improved particle detectors for experiments at ISABELLE.

T. Ludlam
V. Polychronakos

Data Acquisition: Improved systems for data acquisition and on-line monitoring and analysis.

G. Rabinowitz

CONSTRUCTION DIVISION

This Division is responsible for the design and construction of the conventional facilities for the Project.

P. Mohn
E. Dale
J. Feldman
M. Schaeffer
R. Taylor

Physics and Chemistry

Nuclear Physics

Solid State Physics

Atomic and Applied Physics

National Synchrotron Light Source

Chemistry Department

Physics Department

INTRODUCTION

The Physics Department carries out fundamental research in elementary particle (or high energy), nuclear, solid state, and atomic physics. In each discipline, the experimental program is based in large part on Brookhaven's major facilities. These research facilities provide unique capabilities not only to the BNL staff but also to the national scientific community.

Because research in high energy physics is performed by members of the BNL Physics Department, university users, and members of the Accelerator Department, frequently in teams representing more than one group, it seemed best to report that work in a separate section.

The low and medium energy nuclear physics programs carried out by members of the BNL Physics Department and many university community users address questions of the fundamental nature of the structure and interaction of nuclei and nucleons. Beams from the Tandem Van de Graaff Facility, the High Flux Beam Reactor, and the AGS are used in a variety of experiments to study new phenomena. Heavy-ion beams are used for diverse investigations of the reaction mechanisms of heavy ions and the forces between them, the production of the γ-decay of nuclei in states of very high angular momentum, the existence and production of nuclei way off stability, and nuclear electromagnetic properties such as γ-transition rates and static moments. Reactor neutrons are used to perform detailed studies of the structure and dynamics of nuclei utilizing the (n, γ) reaction, as well as for studies of resonance parameters and neutron cross sections of interest to applied fields. The AGS nuclear physics program is concerned presently with the spectroscopy of hypernuclei — nuclei which contain a Λ or Σ hyperon. The Nuclear Theory group has a close interaction with the experimental groups, as well as a wide-ranging program in many exciting topics in nuclear theory. The Laboratory thus provides an opportunity for a very broad program of fundamental nuclear physics. In addition, the Tandem Van de Graaff is used for investigations of the atomic physics of highly excited and stripped atoms.

The solid state research effort is concerned with the cohesive forces that bind atoms together to form the various phases of condensed matter. The facilities such as the High Flux Beam Reactor and the National Synchrotron Light Source, now under construction, provide unique probes for studying the properties of solids on the atomic scale. Particular emphasis is placed on the studies of materials exhibiting phase transformations where a delicate balance of the interatomic forces exists such that a slight change in the external environment (such as temperature or pressure) can produce a significant modification of the atomic arrangement. These studies provide a means of testing the various theories of phase transformations and lead, in many cases, to the prediction of interesting new types of solid structures. Other studies try to unravel the properties of "real" solids, i.e., solids in which the symmetrical arrangement of atoms is disturbed by impurities and crystallographic defects. The resulting changes in the interatomic forces and properties are not always predictable and the experimental results provide a phenomenological understanding of imperfect solids. A further region of growing interest is the study of surfaces. One intriguing problem arising in this field is how the interatomic forces and their arrangement vary when atoms are bound on one side only. Frequently, a different atomic species can be attached to a surface and a new type of atomic arrangement is obtained.

The atomic physics program studies atomic structure and the lifetimes of excited states of highly ionized atoms. Research in applied physics is concerned with measurement of the quantity and location of stable isotopes for a wide variety of problems in solid state physics, biology, medicine, marine science and other fields. Both of these programs make use of the Brookhaven Van deGraaff accelerator facilities and will also utilize the National Synchrotron Light Source when it becomes operational.

At the end of each section a selected list of publications is appended. These lists represent only a small fraction of the papers published during the year.

The two major facilities for experimental nuclear physics research at BNL are the Tandem Van de Graaff accelerator and the High Flux Beam Reactor (HFBR). In addition, research in hypernuclear physics is conducted at the Brookhaven AGS, using secondary beams of kaons. The nuclear theory group supports the experimental effort in both heavy-ion and medium energy physics as well as doing research on other topics of current interest. We present a brief discussion of the highlights of these diverse programs.

THE BNL TANDEM ACCELERATOR

The Tandem Van de Graaff Facility accelerates a number of light and heavy ion beams with good energy resolution over a range of energies. It is utilized by researchers from BNL and numerous other laboratories and universities to conduct basic research in nuclear, solid state, and atomic physics. As new areas of research open up, the Tandem has been continuously upgraded. This trend is continuing with the soon to be implemented accelerating tube extension in MP-7. This modification will upgrade the terminal voltage capability to probably 17 MV or higher. Other recent improvements include a helium-jet system for the study of short-lived radioactivities. The radioactive atoms, produced by bombardment of a target in a gas cell, are swept out of the cell by a helium-aerosol mixture to a tape where the radioactivity is recorded. Beta rays, gamma rays, or delayed protons or alphas can be measured.

A new spectrometer system for high energy γ rays which is based on a large NaI crystal with surrounding photomultiplier tubes typically achieves better than 3% resolution for a 20-MeV γ ray. A large NaI total energy spectrometer for use in various phases of high-spin spectroscopy research is also under design.

A time-of-flight scattering chamber is now in general use. Time resolutions as good as 220 psec have been observed with two-detector systems. A large ion chamber for the measurement of heavy ion energies as well as energy loss has also been incorporated with the time-of-flight system.

The EMS (energy mass selector) system has been considerably improved by augmenting the solid angle to 6 msr, an increase of five times. The EMS now eliminates all of the particles at 0° having the beam energy. By installing a transmission ionization chamber at the end of the EMS, in anticoincidence with the detector, alpha spectra free of background can be obtained. The EMS permits the measurement of evaporation residues as a function of energy, angle, and velocity window through the device, in order to obtain total fusion cross sections.

An ultrasensitive TV imaging system which detects multiple events simultaneously in an X,Y plane and provides an energy measurement and digital coordinates for each event has proven to be a useful device for studies of Coulomb explosion molecular structure and will aid future track or streamer chamber measurements of multiple fragmentation of nuclei.

A proposal to DOE for a cyclotron addition to the Tandem was resubmitted to the Nuclear Sciences Advisory Committee. In this proposal, bunched heavy ion beams from the Tandem are injected into the cyclotron, where they are further accelerated and returned to the present target areas. At its highest energy, the variable energy system will produce beams of 150 MeV/amu oxygen and > 30 MeV/amu uranium. Such an improved facility would greatly expand the range of physics problems which can be addressed at the Tandem.

HEAVY ION EXPERIMENTS AT THE TANDEM

Nuclear physics research with heavy ions is an area of broad interest. Due to the composite nature of the projectile, nuclear reactions induced by heavy ions can involve the transfer of large amounts of angular momentum, energy, and matter. By varying the kinematical conditions, one can study a variety of phenomena: "gentle" processes involving grazing collisions (elastic and inelastic scattering, few particle transfer reactions), or deep inelastic and fusion processes arising from more central collisions. A compound nucleus formed by the fusion of two heavy ions is a very neutron-deficient system at

high excitation energy and high spin. Many states of high spin in known nuclei, and also new nuclei not accessible to other reactions, have been observed in heavy ion reactions.

In the following paragraphs, we review some of the recent experimental results from the Tandem.

Exotic Nuclei: Discovery of ^{21}O

Of the eight so-called "exotic" nuclei with $T_z = +5/2$ which extend from ^{21}O to ^{35}P, only ^{21}O had escaped detection over the past decade. Predictions of masses of these nuclides by early theories were in striking disagreement with experiment and necessitated a reformulation of the theory. Observation of ^{21}O and a measurement of its mass were necessary to complete the set of these eight nuclei with a common relationship. The $^{9}Be(^{18}O,2p)^{21}O$ reaction at 110 MeV bombarding energy for the ^{18}O projectile required nearly the maximum 14-MV terminal voltage and high beam intensity from the BNL tandem accelerator for successful observation of ^{21}O. Radioactive products, including ^{21}O, emerged from a Be foil into a helium gas cell and were swept through tubing to a remote counting location. A unique filtering system removed obscuring radioactivities. A 3.42-second half-life was observed for the ^{21}O activity, and 13 gamma rays were observed in its decay to levels of ^{21}F. The ^{21}O mass-excess was measured through β-γ coincidence measurements, and the observed level structure of ^{21}F was compared with results of shell-model calculations which reproduce its main features in a satisfactory way.

Selective Population of High Spin States in Heavy-Ion Induced Single Neutron Transfer

The use of heavy-ion induced fusion-evaporation reactions has been the principal means for producing residual nuclei in states of very high spin. Most of the information about the yrast and near-yrast structure of nuclei at high spin has come from γ-spectroscopic studies on such reaction-produced nuclei. A complementary approach to such studies has evolved from the demonstration that heavy-ion induced transfer reactions can indeed be used as spectroscopic tools.

A wide-ranging study of the use of heavy-ion induced transfer for spectroscopic studies of nuclei has thus begun. Specifically, the single neutron transfer reactions (^{16}O,^{15}O) and (^{12}C,^{11}C), which have large negative Q values, have been shown to be very selective in populating only high j states in nuclei. These Q values result in rather small cross sections which necessitate the use of high bombarding energies and a large solid angle, highly dispersive spectrometer like the QDDD. The kinematic conditions coupled with the selection rules for transfer give a strong enhancement of high spin states with $j_f = \ell_f + 1/2$ for the (^{16}O,^{15}O) reaction while states with $j_f = \ell_f - 1/2$ are very strong with the (^{12}C,^{11}C) reaction. This is an important feature as the equivalent light-ion reaction, (^{4}He,^{3}He), does not clearly distinguish these states. Coincidence measurements with gamma rays for several isotopes were performed with a specially designed chamber in order to improve the effective energy resolution of the particle experiments. Several nuclei with high-spin states well-established by other experiments were used to determine the reliability of the method while new states have been formed in others. The strong selectivity of the two reactions on the same erbium isotopes is illustrated by the outgoing particle spectra shown in Fig. 1. Note for example the strong increase in the population of the .94 MeV state in ^{169}Er in the (^{12}C,^{11}C) reaction.

Systematics of High Spin Yrast Levels in N = 86 Isotones

The high spin yrast structure of N = 86 isotones ^{150}Gd, ^{154}Er, and ^{156}Yb has been studied in great detail at BNL. Similar studies were carried out on ^{152}Dy at other laboratories.

Interesting systematic trends emerge which include (1) a smooth decrease of the excitation energy of the 2^+ to 8^+ states with increasing proton number, (2) the presence of low-lying negative parity 3^- to 9^- states whose excitation energy increases with increasing proton number, and (3) the regular occurrence of close-lying 10^+ and 11^- states fed by cascades extending to 16^+ and 17^-, respectively. By extending the extreme single particle approach of Kleinheiz, these features may be described as $(f_{7/2})^2$ or $(f_{7/2}h_{9/2})$ neutron configurations coupled to: (1)

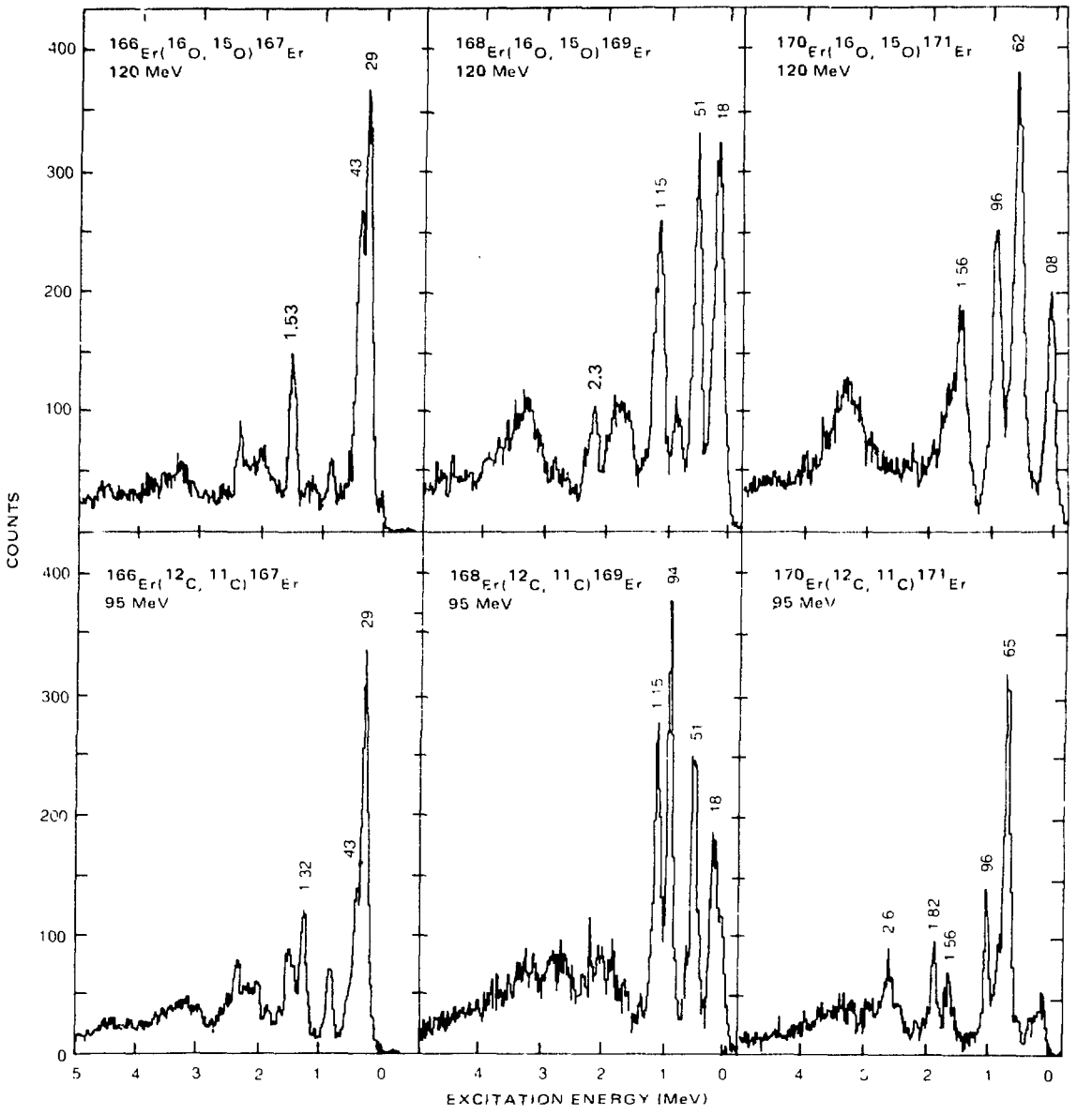

Figure 1. Outgoing particle spectra at 42° from the ^{166,168,170}Er (^{16}O, ^{15}O) (top) and ^{166,168,170}Er (^{12}C, ^{11}C) (bottom) reactions. Excitation energies are listed above the peaks and have an uncertainty of about 0.02 MeV. [P. D. Bond, J. Barrette, C. Baktash, C. E. Thorn, and A. J. Kreiner (submitted to Phys. Rev. Lett.)].

the ground state, (2) a 3$^-$ octupole phonon, and (3) to $[(i_{13/2})^2]_{10}^+$ or $(i_{13/2}h_{9/2})_{11}^-$ configurations. The near equality of the transition energies, however, may indicate admixtures of some quadrupole vibrations in the wave functions.

Since maximal alignment of 4 neutrons in this region cannot generate more than ~20 h units of angular momentum, proton excitation becomes necessary for states with $J > 20$. Interestingly, in ^{150}Gd, ^{152}Dy (^{154}Er), a sequence of transitions, starting with $J^\pi = 21^-(19^-)$, decreasing in energy, establishes a quasiband structure up to $J^\pi = 27^-(25^-)$. Moreover, the energy spacings within these structures closely resemble the $[(f_{7/2})^2]_{0^+,2^+,4^+,6^+}$ energy spacings of their corresponding N = 84 isotopes. Both the

lifetimes of the 21$^+$ state in ^{152}Dy ($T_{1/2}$ = 14 nsec) and 19$^+$ state in ^{154}Er ($T_{1/2}$ = 460 psec) indicate transition rates of ~1 Wu for the analogous 21$^+$ → 19$^+$ and 19$^+$ → 17$^+$ transitions in the respective nuclei. Such correlations are suggestive of coupling a $(\nu f_{7/2})^2$ two-neutron structure to bandheads composed of $[(\pi h_{11/2})^2]_{8^+,10^+}$ $(\nu h_{9/2}\, \nu i_{13/2})_{11}$ aligned shell-model configurations. The presence of readily recognizable $(j)^2$ configurations in this region suggests that even at spins up to 30, relatively pure and near-spherical shell model states persist as prominent components in the excitation. See Fig. 2.

High-energy Gamma Decays to Intermediate States

The ^{12}C(α,γ)^{16}O reaction has been studied with the highest energy beams available from the MP-7 tandem. Resonances near 40-MeV excitation in ^{16}O were observed to decay by emitting a single high-energy gamma ray. The final state, the first 6$^+$ level of ^{16}O at 14.8 MeV, has an alpha-cluster configuration with a high degree of symmetry and is simply described by the SU$_3$ model. Comparisons with shell model calculations suggest that the observed resonances are the 8$^+$ components of a Giant Quadrupole vibration of the first 6$^+$ state in ^{16}O. This represents the first possible example of a Giant Quadrupole Resonance built on an excited state in any nucleus. Furthermore, the structure is fundamentally different from the Giant Resonance built on the ground state since the 6$^+$ parent state has a structure very different from the ground state.

Selected Publications (Tandem)

D. E. Alburger, C. J. Lister, J. W. Olness, and D. J. Millener. Beta decay of ^{21}O. *Proc. Intern. Conf. on Nuclear Physics, Berkeley, California, August 24-30, 1980*, Vol. 1, p. 149; *Phys. Rev.* C (in press).

C. Baktash, E. der Mateosian, O. C. Kistner, A. W. Sunyar, D. Horn, and C. J. Lister. Evidence for near-spherical shell model structure in the high spin states of N = 86 isotones. *Proc. Intern. Conf. on Nuclear Physics, Berkeley, California, August 24-30, 1980*, Vol. 1, p. 323.

P. D. Bond. Polarizations in heavy-ion induced transfer reactions. *Phys. Rev.* **C 22**, 1539-1549 (1980).

P. D. Bond and J. Barrette. Location of high-J orbital two-quastiparticle states in Sm and Nd isotopes. *Proc. Intern. Conf. on Nuclear Physics, Berkeley, California, August 24-30, 1980*, Vol. 1, p. 380.

A. C. Dirienzo, H. A. Enge, S. B. Gazes, M. K. Salomaa, A. Sperduto, W. Schier, and H. E. Wegner. New isotope ^{199}Rn and evidence for an isomeric state ^{199}Rn^m. *Phys. Rev.* **C 21**, 2101-2102 (1980).

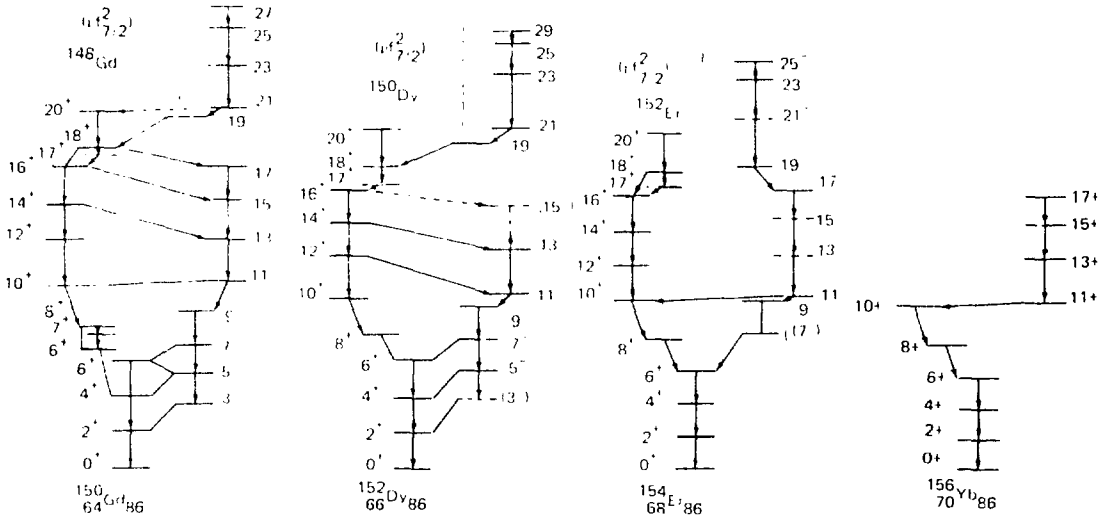

Figure 2. Systematics of yrast energy levels of N = 86 isotones ^{150}Gd, ^{152}Dy ^{154}Er and ^{156}Yb. The dots adjacent to the 21$^+$ to 27$^+$ states in ^{150}Gd, ^{152}Dy, and to the 19$^+$ to 25$^+$ states in ^{154}Er, indicate the 0$^+$ to 6$^+$ level energies in the (N-2) isotopes relative to the 21$^+$ (19$^+$) states as bandheads. [C. Baktash, E. der Mateosian, D. Horn, O. C. Kistner, C. J. Lister, and A. W. Sunyar (to be published)].

G. GOLDRING, Y. EISEN, P. THIEBERGER, H. E. WEGNER, AND A. FILEVICH. C_3 + NCO molecular ion structure studies by Coulomb explosion. *Phys. Rev.* A (submitted).

D. HORN, G. R. YOUNG, C. J. LISTER, AND C. BAKTASH. High spin particle states in ^{152,153}Er. *Phys. Rev.* C (in press).

A. J. KREINER, A. FILEVICH, G. GARCIA BERMUDEZ, M. A. J. MARISCOTTI, C. BAKTASH, E. DER MATEOSIAN, AND P. THIEBERGER. High spin band structure of ^{192}Tl. *Phys. Rev.* **C 21**, 933-939 (1980).

A. J. KREINER, M. A. J. MARISCOTTI, C. BAKTASH, E. DER MATEOSIAN, AND P. THIEBERGER. High spin structure of ^{75}Br and the (N,Z) dependence of the nuclear deformation in the Br region. *Phys. Rev.* C (in press).

C. J. LISTER, D. E. ALBURGER, P. E. HAUSTEIN, AND J. W. OLNESS. The new isotope ^{81}Yb and mass systematics of neutron deficient yttrium isotopes. *Bull. Am. Phys. Soc.* **25**, 603 (1980).

A. M. NATHAN, A. M. SANDORFI, AND T. J. BOWLES. Intermediate structure observed in the radiative capture of ^{12}C by ^{12}C near the Coulomb barrier. *Phys. Rev.* C (submitted).

A. M. SANDORFI, J. R. CALARCO, R. E. RAND, AND H. A. SCHWETTMAN. Fission modes in ^{24}Mg. *Phys. Rev. Lett.* **45**, 1615-1618 (1980).

T. P. SJOREEN, D. B. FOSSAN, U. GARG, A. NESKAKIS, A. R. POLETTI, AND E. K. WARBURTON. High-spin states in ^{205}At. *Phys. Rev.* C (submitted).

J. S. VAAGEN, D. L. HILLIS, P. D. BOND, C. E. THORN, M. J. LEVINE, J. J. KOLATA, C. FLAUM, AND J. C. SENS. Striking sensitivity to the nuclear hexadecapole parameter inferred from the angular distribution of ^{12}C + ^{184}W (4$^+$) at a carbon energy of 70 MeV. *Phys. Lett.* **91B**, 361-364 (1980).

THE HIGH FLUX BEAM REACTOR

The High Flux Beam Reactor (HFBR) at Brookhaven provides a variety of neutron beams for solid state and nuclear structure studies. The beams used for nuclear measurements at the HFBR consist of both pulsed beams for time-of-flight measurements and continuous beams filtered through various materials or diffracted from crystal planes. Both "white" and monoenergetic beams are available with energies up to 24 keV. These beams are used for (n, γ) reaction studies, production of fission products, and cross section measurements.

The (n, γ) reaction is capable of populating a wide variety of final nuclear configurations, and thus provides a powerful tool in nuclear structure studies. Coincidence and angular correlation measurements of the resulting γ-ray cascade can provide spin and parity assignments for excited levels. Using the technique of average resonance capture, a nonselective reaction, a complete set of low spin states can be populated. The completeness of the level schemes is an important feature, which enables one to test nuclear models in great detail.

During 1979, the on-line isotope separator TRISTAN was installed at the reactor. This facility provides beams of fragments resulting from the fission of ^{235}U. These neutron-rich nuclides are used for studies of delayed neutron emission and systems far off the valley of stability. Active participation in TRISTAN experiments has involved representatives from several laboratories and universities. On-going developments in ion source technology have permitted fragment activities with lifetimes as short as 0.05 sec to be measured. The capabilities of TRISTAN are further enhanced by the installation of a multidetector angular correlation system. A long-term goal for TRISTAN remains to make use of the high HFBR flux through an internal target.

In the next few sections, we review some of the highlights of the research program at the HFBR.

Level Structure of ^{168}Er: A Comparison to IBA Model Predictions

The recent proposal and testing of the IBA model is a most significant development in nuclear structure physics. This model attempts to provide a simple and yet comprehensive interpretation of the collective excitations in widely diverse nuclei spanning much of the periodic table. It is complementary to previous models but capable of incorporating the key aspects of many of them within a single framework.

Despite remarkable success in nuclei ranging from Se to Pt, the model has generated controversy concerning its basic theoretical foundations. These controversies now center on the question of its ability to account for the properties of deformed nuclei, a class of nuclei for which the model, surprisingly, has never been thoroughly tested. By exploiting the unique capabilities of the nuclear physics facilities at the BNL High Flux Beam Reactor to disclose com-

plete sets of nuclear levels, an exhaustive study of ^{166}Er has recently been completed in collaboration with the Institut Laue Langevin in Grenoble, France, where likewise unique but complementary facilities exist. The remarkably complete level scheme developed for this deformed nucleus displays a characteristic set of gamma-ray transitions (β-band to γ-band transitions) that are predicted by the IBA but forbidden in other models. IBA calculations were caried out and compared with the data. Overall, excellent agreement with the data was obtained. The results for energy levels are shown in Fig. 3. Stimulated by these results and the controversy surrounding the model when applied to deformed nuclei, several groups are now reexamining the relation of the IBA to geometrical models as well as extensions of those models to generate similar predictions. New insights into the structure and character of the collective states predicted by the IBA and of the relation of this group theoretic model to geometrical ones which describe collective excitations in terms of shape changes of the nucleus may emerge.

Beta-delayed Two-neutron Emission from ^{98}Rb

While multiple neutron decay of light elements such as ^{11}Li and ^{30,31,32}Na has been previously reported, no such phenomenon has been reported for a *fission* fragment. A neutron-neutron time correlation technique was employed to search for two-neutron emission in ^{98}Rb, which has an energy excess $Q_\beta - Q2N \approx 1.82$ MeV. The ^{98}Rb data were obtained at the isotope-separator on-line TRISTAN at BNL using a neutron detector of 40 tubes of ^{3}He embedded

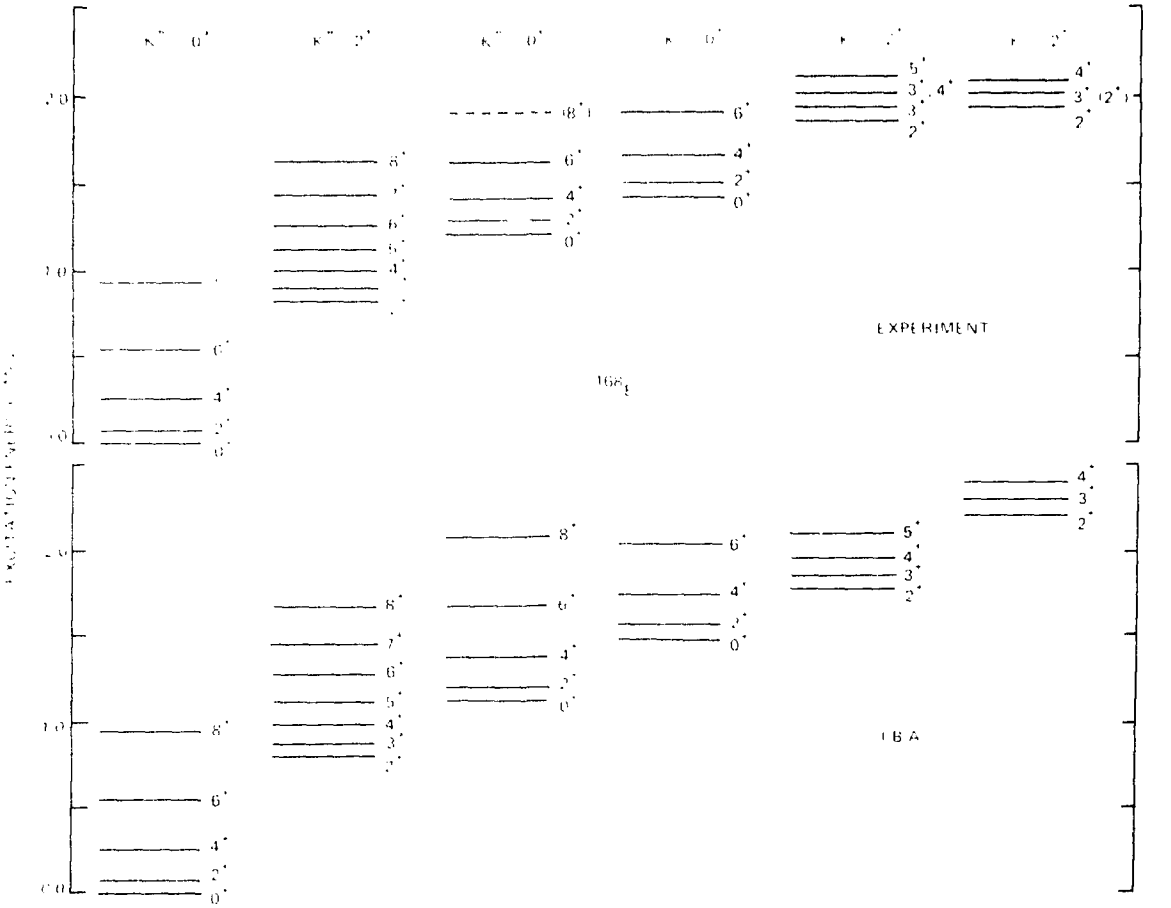

Figure 3. Levels in ^{166}Er compared with the results of the IBA calculation for 16 bosons. Only experimental bands below the pairing gap, estimated as ~ 2 MeV, have been included. [D. D. Warner, R. F. Casten, and W. F. Davidson, *Phys. Rev. Lett.* **45**, 1761 (1980)].

in polythene. The pulses from this detector were passed to an interval analyzer which records the distribution of time intervals between successive events. The time distribution shows an excess near t = 0 corresponding to two-neutron emission with a probability of $P_{2N} \sim 0.025\%$. A search for other multiple neutron emitters is being made, and a similar effect is seen for ^{99}Rb.

Low-Lying 0^+ States in Transitional $^{112-116}$Ce Nuclides

Nuclear fission produces a variety of isotopes on the neutron-rich side of stability. Nuclear models are tested by examination of the effect of varying neutron number, A − Z, across a series of particular isotopes. Of special interest are those nuclides in a transitional region between rotators and vibrators. TRISTAN has allowed a detailed study in such a region, namely in the area from A = 140 to A = 150, for isotopes of Ce. The IBA model provides a good description of levels in the even A Ce isotopes, particularly in the position of the first excited 0^+ levels. These levels are a sensitive indicator of nuclear structure. The results show that the onset of deformation in Ce occurs at an intermediate neutron number between that observed in the Ba isotopes and that observed in the rare earth isotopes like samarium and gadolinium.

Selected Publications (HFBR)

R. F. CASTEN. Survey of experimental test of the IBA model. *Nucl. Phys. A347,* 173 (1980).

R. F. CASTEN, D. D. WARNER, M. L. STELTS, AND W. F. DAVIDSON. Consequences of completeness in nuclear spectrosocpy. *Phys. Rev. Lett.* **45,** 1077 (1980).

R. E. CHRIEN. "Investigating the nucleus by neutron radiative capture," in *A Festschrift for Maurice Goldhaber, July 25, 1980, Transactions of the New York Academy of Sciences.* G. Feinberg, A. W. Sunyar, and J. Weneser, Eds. Series II, Vol. **40** (1980), p. 40.

R. E. CHRIEN, M. L. STELTS, V. MANZELLA, R. GILL, F. WOHN, AND J. C. HILL. "TRISTAN-II at Brookhaven." In *Nuclear Spectroscopy of Fission Products,* Till von Egidy, Ed. The Institute of Physics, Bristol and London (1980), p. 44.

P. L. REEDER, R. A. WARNER, T. R. YEH, R. E. CHRIEN, R. L. GILL, M. SHMID, H. I. LIOU, AND M. L. STELTS. Beta-delayed two-neutron emission from the fission product nuclide ^{98}Rb. (To be published.)

W. B. WALTERS, U. CHUNG, F. K. WOHN, K. SISTEMICH, H. YAMAMOTO, D. BRENNER, R. L. GILL, H. SHMID, H. I. LIOU, M. L. STELTS, G. M. GOWDY, Y. Y. CHU, AND R. E. CHRIEN. Angular correlation studies of the low-lying 0^+ states in transitional $^{112-116}$Ce nuclides. *Bull. Am. Phys. Soc.* **26,** 552 (1981).

D. D. WARNER, R. F. CASTEN, AND W. F. DAVIDSON. A detailed test of the IBA in a well deformed nucleus: the positive parity states of ^{166}Er. *Phys. Rev. Lett.* **45,** 1761 (1980).

Medium Energy Physics

The major thrust of the intermediate energy physics program at BNL is the study of nuclear structure by using energetic elementary particles as probes. The intense separated kaon (K^-) beam available at the BNL Alternating Gradient Synchrotron (AGS) has been used to study the formation of "hypernuclei." This new nuclear species is created when a K-particle transfers its "strangeness" to a neutron in the nucleus, converting it into a lambda hyperon (Λ) via the (K^-, π^-) reaction. A focusing magnetic spectrometer measures the kaon momentum (800 MeV/c) to 0.2%. A second magnetic spectrometer can rotate to detect outgoing pions from hypernuclear formation at angles up to 35° with respect to beam direction. The observed kaon and pion momenta determine the energy of the hypernuclear state. The overall energy resolution with the thick (2 g/cm^2) targets was about 2.2 MeV. Particle trajectories measured by multiwire proportional chambers provide constraints for rejection of background which results primarily from two-body kaon decay. The rotation of the spectrometer permits angular distribution measurements for the outgoing pion, which are essential for spin assignments.

A program for making improvements in the spectrometer continues, with the aim of augmenting the event rate substantially by increasing the kaon flux incident on the target

and also the solid angle of the pion spectrometer. The larger event rate permits detection of hypernuclear γ rays in coincidence with pions, thereby obtaining more spectroscopic information.

A workshop group formed for the purpose of designing a new high intensity kaon facility at BNL drew up a list of performance specifications for the facility. The workshop meetings were attended by a number of potential users from the University community, who also participated in the design. The main goals of such a facility are to attain an event-rate increase of 100 and a spectrometer resolution of a few parts in 10^4. Many types of experiments with cross section of the order of 1 μb/sr then become feasible.

Proton projectiles were also used at the High Resolution Spectrometer (HRS) at the Los Alamos Meson Physics Facility (LAMPF), in collaboration with several other groups, in a study of Giant Resonances excited by inelastic scattering of 800-MeV protons.

We now discuss the highlights of the experimental medium energy program during the last year.

Hypernuclear Excited States

Last year, $^{12}_{\Lambda}$C was studied by means of the (K^-, π^-) reaction on ^{12}C. Spin-parity assignments were deduced from the angular distributions to various final states of $^{12}_{\Lambda}$C. This year, in further experiments at the Brookhaven AGS, excited states of the hypernucleus $^{13}_{\Lambda}$C have been observed for the first time. In addition, two new hypernuclear species, $^{15}_{\Lambda}$O and $^{11}_{\Lambda}$N have been identified.

The spectrum of $^{13}_{\Lambda}$C has been measured over a range of momentum transfer from 50 to 330 MeV/c. Different hypernuclear states are excited preferentially as the momentum transfer is varied. For the $^{13}_{\Lambda}$C measurement a scintillation counter was fabricated consisting of benzene containing carbon enriched to 99% ^{13}C. The scintillation counter target provides strong background suppression by making use of the large signal produced by the decay of the hypernucleus. This unique target made it possible to take data at angles where hypernuclear formation and kaon decay are kinematically indistinguishable.

Excitation spectra of $^{13}_{\Lambda}$C were measured at spectrometer settings of 0°, 5°, 10°, 15°, and 25°. The spectrum observed at small angles (0° and 5° samples combined) exhibits five distinct peaks in contrast to the case of $^{12}_{\Lambda}$C, where only two peaks were observed. The two $^{13}_{\Lambda}$C peaks correspond to binding of the Λ in s and p states (separated by 10.8 MeV) to a ^{11}C core in its ground state.

In the case of $^{13}_{\Lambda}$C, the reaction strength goes primarily into core excited states, which, by virtue of the T = 1/2 isospin of the ^{13}C target, may be hypernuclear states with either T = 0 or T = 1. Further, the excitation spectrum of the ^{12}C core should exhibit similarities to that observed in (p,d) reactions on ^{13}C, where a neutron is similarly removed. Five states, the 0^+, T = 0 ground state, the 4.44-MeV 2^+, T = 0, the 12.71-MeV 1^+, T = 0, the 15.11-MeV 1^+, T = 1 and the 16.11-MeV, 2^+ T = 1 state are known to dominate the spectrum in the (p,d) reaction on ^{13}C at 55 MeV.

The five peaks observed in $^{13}_{\Lambda}$C may now be interpreted. The first corresponds to the $^{13}_{\Lambda}$C ground state (Λ in an s orbit, bound to the ^{12}C unexcited core). The second peak at 4.45 MeV arises from the Λ in the s orbit bound to the 2^+, T = 0 excited ^{12}C core. Peak three at 10.41 MeV is separated from the $^{13}_{\Lambda}$C ground state by about the Λ p-s excitation energy in $^{13}_{\Lambda}$C and is interpreted as a p orbit Λ bound to the ground state ^{12}C core. Peak four at 16.39 MeV is similarly identified as a p orbiting Λ bound to an excited (4.44-MeV, 2^+, T = 0) ^{12}C core. Peak five at 25.71 MeV excitation is interpreted as an unresolved composite peak consisting of a Λ in the p state coupled to the ^{12}C core isospin excitations near 15 and 16 MeV. Excitation spectra taken at different angles where momentum transfer differs not only lead to excitations of different hypernuclear states but also to conclusions about the magnitude of the Λ spin-orbit splitting and the Λ-nucleus residual interaction. Further, preliminary experiments with γ-rays observed in coincidence with peak two and not with peak one not only support the state interpretations but also suggest that development of hypernuclear gamma-ray spectroscopy may be forthcoming.

Selected Publications (Medium Energy Physics)

M. MAY, S. CHEN, R. E. CHRIEN, D. MAURIZIO, H. PALEVSKY, R. SUTTER, Y. XU, P. BARNES, B. BASSALLECK, R. EISENSTEIN, R. GRACE, P. PILE, R. RIEDER, W. WHARTON, M. DEUTSCH, J. PIEKARZ, S. BART, E. V. HUNGERFORD, R. HACKENBERG, B. MAYES, L. PINSKY, H. PIEKARZ, R. CESTER, AND R. L. STEARNS. Observation of Excited States of the Hypernuclei $^{13}_{\Lambda}$C, $^{14}_{\Lambda}$N and $^{15}_{\Lambda}$O. To be published.

R. L. STEARNS, R. E. CHRIEN, R. J. SUTTER, T. J. KRIEGER, H. I. LIOU, AND T. KOZLOWSKI. Giant Resonances Excited by Scattering of 800 MeV Protons. *Proc. Intern. Conf. On Nuclear Physics, Berkeley, California, August 24-30, 1980,* Vol. 1, p. 248.

Nuclear Theory

The nuclear theory group at BNL functions in a mode of strong interaction among its members and also with experimentalists at this laboratory. In addition, extensive cooperation exists between group members and scientists at other institutions or in the other theoretical disciplines at Brookhaven.

Activities of the nuclear theory group have recently included studies of heavy-ion induced reactions, especially in relation to experimental activity here and elsewhere, investigations of nuclear structure on its own and in extraction of structure information from electron-nucleus, π-nucleus, or nuclear γ-decay experiments. Such activities also involve an array of intermediate energy reactions for which experimental data are presently being gathered; in particular the hypernuclear structure-physics opening up by recent experiments on the (K^-,π^-) reaction. Further, close contact is maintained with the nuclear chemistry group at BNL which experimentally defined, and continues to explore, the solar neutrino puzzle. Direct and consequential effort has recently been expended in ccoperation with experimentalists to design a cyclotron post-accelerator for the BNL MP Tandems and to study possible π, K beam lines at the AGS.

Selected highlights of the past year are now discussed.

Massive Heavy Ion Scattering

A project that is just now coming to fruition is the development of coupled channels calculations for reactions induced by massive heavy ions. A variation on the inward-outward method of solving coupled Schroedinger equations has been developed which facilitates calculations for massive heavy ion reactions in which many channels are involved. Application has already been made to inelastic scattering calculations for existing data on ^{40}Ar + ^{238}U and ^{84}Kr + ^{209}Bi, above the Coulomb barrier. A dominating effect of multiple Coulomb inelastic excitation above the barrier has been exhibited. A sub-Coulomb test case of 340 MeV Kr on ^{238}U Coulomb exciting up to the 24^+ state of ^{238}U (169 channels) exhibits the proper quantum mechanical differences from the semi-classical calculation.

Hypernuclear Physics

The main thrust of current research is in hypernuclear structure physics. Experimental data on hypernuclear spectra and γ transitions are becoming more abundant. These data require interpretation. In particular, the (K^-, π^-) reaction has been exploited by experimental groups at CERN and BNL to produce an impressive array of excited Λ-hypernuclear states, $^{12}_{\Lambda}$C, $^{13}_{\Lambda}$C, $^{14}_{\Lambda}$N, $^{15}_{\Lambda}$O, $^{16}_{\Lambda}$O, as well as heavier and lighter nuclei, and perhaps also Σ-hypernuclei. Preliminary experiments on γ-ray transitions between such states has elevated hopes for a greatly improved spectroscopy. Several theoretical efforts at BNL on explicit calculations of the reaction mechanism have permitted preliminary description of the structure. More recently a complete structure calculation, using as a basis weakly coupled Λ-nuclear-core states, has been developed and already indicates several surprises: what appears to be direct empirical evidence for simple weak coupling in fact conceals the possibility of strong coherences.

Anti-nucleon Interactions with Nuclei

The new LEAR (Low Energy Antiproton Ring) project at CERN, which will provide in-

tense low momentum (150-600 MeV/c) antiproton beams, may revolutionize the field of experimental antinucleon physics. The group is engaged in trying to predict some new phenomena which may be found in the next generation of $\bar{N}$ experiments. In $\bar{p}$-nucleus scattering, single particle resonances may occur which are not simply reflections of a basic $\bar{N}N$ two-body resonance or bound state. The signature of this "orbiting" phenomenon is peaking in the 180° excitation function for $\bar{p}$ elastic scattering. Thus far $\bar{N}$-nucleus interactions are largely unexplored, either theoretically or experimentally. This field seems ripe for the discovery of new phenomena.

Stellar Collapse

Work is in progress on collaborations in astrophysics with scientists at SUNY, Stony Brook. A hydrodynamical model of stellar collapse is unable to produce a viable shock wave after bounce. The shock dies before the star's mantle is blown off. Some changes in the nuclear matter equation of state at high density may overcome this difficulty.

Selected Publications (Nuclear Theory)

E. H. AUERBACH, C. B. DOVER, AND S. H. KAHANA. Resonance phenomena in antiproton-nucleus scattering. *Phys. Rev. Lett.* **46**, 702 (1981).

A. J. BALTZ, B. V. CARLSON, AND M. S. HUSSEIN. Multiple Coulomb polarization potential for heavy ion scattering. Accepted for publication in *Phys. Lett.*

A. GAL AND C. B. DOVER. Narrow Σ-hypernuclear states. *Phys. Rev. Lett.* **44**, 379 (1980).

S. H. KAHANA, T. MAZOUREK, AND G. COOPERSTEIN. Neutrinos and stellar collapse. *1980 Dumand Proceedings*, University of Hawaii.

Solid State Physics

INTRODUCTION

The solid state physics effort is mainly involved with understanding the physical, electronic, and magnetic properties of condensed matter. These properties can be studied in a number of different experimental conditions, e.g., temperature, pressure, and defects, by a variety of unique probes available at Brookhaven. These probes encompass various energy photons, neutrons, protons, electrons, and positrons. All of these tools help provide complementary information about the properties of solids.

The main solid state facility presently used at Brookhaven is the High Flux Beam Reactor (HFBR) which provides an intense beam of low energy neutrons. These neutrons are used in measuring the motion and positions of atoms and the magnetic nature of condensed matter. The National Synchrotron Light Source (NSLS), another major facility, is nearly operational. This facility will provide intense sources of tunable infrared, ultraviolet, and x-ray radiation which can be used to probe atomic and electronic properties of solids and their surfaces. A major portion of the ongoing research is concerned with the development of equipment and gaining experience so that full use can be made of the NSLS when it is completed. Other facilities are also available that can probe the arrangement of the atoms or produce disorder, i.e., defects, by irradiation, which is known to produce large changes in both electrical and physical properties.

NEUTRON SCATTERING STUDIES

Thermal neutrons are an ideal probe for measuring positions and motion of atoms in condensed matter. This is because thermal neutrons have wavelengths comparable to interatomic spacings and energies comparable to the elementary excitations of the solid. Additionally, the magnetic moment of the neutron can interact directly with the magnetic moment associated with unpaired electrons, so the neutron is an ideal probe of the magnetic nature of

solids. The HFBR provides an intense beam of thermal neutrons which allows for the study of a wide variety of problems. The following examples represent only a few of the problems presently being studied at the HFBR.

Spin Glasses

A spin glass can be defined as a magnetic system, usually a metallic alloy, which is characterized by a freezing of the spins in a random arrangement such that there is no long-range magnetic order. The randomness of the spin direction is analogous to the random order occurring in amorphous structures such as glasses and thus, the term spin glass. These systems differ considerably from conventional ferromagnetic materials such as iron where, at low temperatures, the spins are frozen, but they all point in the same direction. By judiciously choosing the alloy composition, an interesting sequence of phases occurs upon decreasing temperature. At high temperatures, all the spins are fluctuating in a random manner due to the thermal energy. Little correlation exists amongst the spins and the system behaves as a paramagnet. As the temperature is lowered, correlations develop and a magnetically ordered state exists. On lowering the temperature further, the ordered magnetic state begins to break up and the magnetization decreases to a small value. The onset of ferromagnetic order in solids is reasonably well understood; however, the cause for the breakup of this order is not known. Our goal has been to probe these systems microscopically with thermal neutrons. By inelastically scattering neutrons off the collective excitations of the spin system, we obtain information about the interactions between the spins. A study of the alloy Fe_xCr_{1-x} with $x = 0.26$ yielded an interesting behavior of the spin-wave energy. Well-defined excitations are observed in the ferromagnetic regime and as T is lowered, the frequency of the excitations decreases. This contrasts strongly with normal ferromagnetic materials where the frequency of the excitations continues to increase as the spins become more and more ordered.

Magnetic Superconductors

A number of ternary compounds become superconducting even though they contain a chemically ordered sublattice of magnetic rare-earth ions. Studies of the physical properties of these materials have revealed anomalies below a temperature, T_c, which have been attributed to magnetic ordering transitions. Using neutrons it has been demonstrated that simple magnetic structures with long-range order occur, and some of the magnetic structures have been solved. It has been found that in $DyMo_6S_8$ and $TbMo_6S_8$, for example, an antiferromagnetic structure coexists with superconductivity. In other compounds, such as $ErRh_4B_4$ and $HoMo_6S_8$, the development of ferromagnetism is responsible for the quenching of superconductivity. Small angle neutron scattering experiments show that, near the transition from superconductor to ferromagnet in these two compounds, additional scattering occurs with peaks at a finite wave vector. The temperature and wave vector dependence of the scattering demonstrate that an oscillatory magnetic structure has formed. The competition between ferromagnetism and superconductivity produces this compromise long-wavelength oscillatory state at intermediate temperatures. Further development of the magnetic state with decreasing temperature results in destruction of the superconductivity, and the compounds are pure ferromagnets at low temperature.

SPECTROSCOPY OF SOLIDS

With the NSLS due to become operational in the near future, the development of new techniques and equipment, as well as the modification of old techniques, has been the major emphasis of this effort. An example is given below on what new physics can be performed with high brilliance x-ray sources.

X-ray Scattering

In recent years, developments in high brilliance x-ray sources, such as high power rotating anode generators and electron storage rings for synchrotron radiation applications, have permitted considerable improvement in the momentum resolution achievable in scattering experiments. A momentum resolution of $\Delta Q \sim 10^{-1}$ Å^{-1} can be reached with the new types of x-ray sources. In fact, one can now think realistically of carrying out experiments in a resolution range of 10^{-5} to 10^{-6} Å^{-1} at the National Synchrotron Light Source (NSLS). Such high resolution measurements are very useful in determining small variations in atomic arrange-

ments in materials, such as the structural changes associated with a phase transition or disorder arising from particular types of lattice defects.

The x-ray scattering study discussed here was carried out on the pseudobinary alloy system $Nb_3Sn_{1-x}Sb_x$, using a rotating anode x-ray source with a resolution in momentum of about 10^{-1} Å^{-1}. Complementary scattering measurements were also made using neutrons at relatively low resolutions (10^{-3} Å^{-1}) in order to confirm that the effects seen with x-rays were truly characteristic of sample bulk, rather than arising from near-surface scattering (the absorption of neutrons is generally much lower than that of x-rays), and to map out the general features of the phase diagram.

The $Nb_3Sn_{1-x}Sb_x$ alloys are high temperature superconductors with basic crystal structures of the *A*15 type. These materials are cubic at ordinary temperatures, but undergo martensitic phase transitions with tetragonal distortions at low temperatures. Lattice instabilities during these phase transitions in the intermetallic compounds have been of considerable interest since it is thought that these are related to the onset of superconductivity. The $Nb_3Sn_{1-x}Sb_x$ system is of particular interest because opposite tetragonal distortions ($a > c$ and $a < c$) have been observed in the Sb concentration range $x = 0$ to 0.15.

The initial survey by neutron scattering demonstrated that the reversal in tetragonal distortion is not a gradual concentration-dependent effect, but rather that there are two distinct tetragonal phases, as shown in Fig. 1. The high-resolution x-ray studies were concentrated on the boundary between these tetragonal phases. Other systems with two tetragonal phases commonly have an intervening orthorhombic phase separating the two phases with opposite tetragonality. Investigation this possibility required this high resolution of 10^{-1} Å^{-1}.

The x-ray measurements yielded well-separated Bragg peaks. This separation allowed unambiguous tetragonal assignments as the temperature was changed through the phase boundary, and the exclusion of an intervening third phase. These measurements also established the first-order nature of this transition. Moreover, it was possible to determine the sublattice displacements of Nb atoms which develop so as to maintain Nb positioning at the center of a distorted tetrahedron of Sn(Sb) nearest neighbors, regardless of the sign of tetragonal distortion.

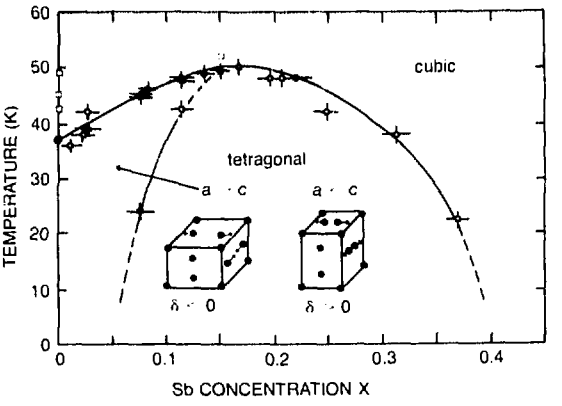

Figure 1. Phase diagram of the pseudobinary alloy $Nb_3Sn_{1-x}Sb_x$. The present results on the phase boundaries of the martensitic cubic-to-tetragonal and the newly observed tetragonal-to-tetragonal phase transitions are represented by black circles. White circles and squares represent previous measurements on similarly grown specimens and RCA crystals, respectively. Tetragonal distortion and sublattice displacement, which were found to be uniquely correlated, are schematically shown for both tetragonal phases.

SOLID STATE THEORY

In order to best utilize our unique experimental facilities theorists work closely with experimentalists on a number of problems. These include phase transitions, bulk and surface electronic properties including defects and, increasingly, because of the National Synchrotron Light Source, the interaction of light with matter. The work on phase transitions and critical phenomena relies on renormalization group and field-theory techniques while electron energy band theory is being employed increasingly in bulk and surface studies.

Heats of Formation of Alloys

An understanding of the energetics of alloy formation is of importance. Recently, a simple electron band theory model was used to predict the heats of formation of binary transition metal alloys at equiatomic composition. This model is essentially a Friedel scheme where the energetics is entirely associated with d band

electrons and the parameters of interest are the centers of gravity of the d bands, the band widths, and the number of electrons occupying the bands. The model presumes a disordered system, and does not depend on crystallographic structure. A problem confronting any simple scheme of alloy formation is that of dealing self-consistently with charge transfer between atomic sites. This was dealt with approximately by placing the two constituent species of atoms into the alloy lattice and, prior to letting them interact, bringing their local chemical potentials to a common value. Using a physically plausible set of band parameters, one was able to reproduce the heats of formation of the sixty alloy systems, for which there are data, with an rms error of 0.06 eV/atom. This is less than the rms experimental uncertainty and about equal to the spread in heats associated with the varying crystallographic structures actually encountered in the alloys. It would appear that Friedel's simple description of the transition metals provides quantitative as well as qualitative insight into transition metal alloy formation.

PARTICLE-SOLID INTERACTION PHYSICS

Lattice defects and disorder play major roles in determining the macroscopic properties of solids. Atomic particles can be employed to create disorder in solids or to study it.

Particle-solid interaction physics entails the use of high- or low-energy particles such as positrons, electrons, heavy ions, or neutrons for each of these purposes. The examples to follow represent two methods to use these probes as tools of basic research, and illustrate the kinds of information that can be obtained from their application.

Slow Positron Beam Research

With the newly developed capability of producing a high-intensity variable energy (0-10 keV) positron beam, research in the positron effort has developed in a new direction. Increased moderator efficiency, i.e., conversion of fast positrons emitted from a radioactive source to monoenergetic positrons (~1eV), opens the door to new experiments in many areas of physics. In the past two years, moderator efficiency has increased by over two orders of magnitude. We have recently shown that when Cu was evaporated epitaxially on a W(110) crystal, one can expect a moderator efficiency of approximately 1%. Brookhaven presently has both a magnetic and electrostatic positron beam operating in ultra-high vacuum conditions. These unique beams are presently being utilized in the study of surfaces, interfaces, and thin films in both metals and semiconductors.

An example of one kind of experiment involving germanium and silicon crystals has opened an exciting new avenue of investigation of the mechanisms which determine the mobility of positrons (and analogously, holes) in these materials. Charge carrier motion is, of course, central to the semiconductor technology. The more fundamental interest is in the details of the processes which control this motion. From this viewpoint, the question of whether a charge carrier is behaving as a quantum-mechanical wave packet or a classical particle becomes important, although experimental insight into this problem has been difficult and elusive.

The mobility of positrons has been measured in both Ge and Si as a function of temperature and crystallographic direction. The results indicate that the positron abruptly changes its configuration from an extended wave-like entity at low temperatures to become a localized small particle above ~850K in Ge. Once the positron enters the localized state, it diffuses much more slowly.

Materials Synthesis and Characterization

Another example is concerned with structural chemistry and crystal structure determination of solids—an important aspect of solid state physics and materials research. For several decades, x-ray, and, more recently, neutron diffraction techniques have been the cornerstone of structural studies. Single crystals are normally used in these studies, since polycrystalline samples tend to give more complicated diffraction patterns with many overlapping peaks. They are, however, generally much easier to synthesize. In the last decade there has been a notable renaissance in neutron powder structure determination which involves fitting of a structural model to the whole diffraction pattern.

This profile refinement technique has been applied to neutron data collected at the HFBR from a number of polycrystalline inorganic

compounds. Typical examples of compounds recently studied are the mixed oxide system formed between $BaBiO_3$ and $BaPbO_3$, in which a novel type of superconducting phase is found, and $LiMoO_2$, which is one of a series of lithiated oxides under investigation as battery electrode materials.

In contrast to the neutron case, profile refinement of x-ray powder data is still in its infancy, mainly because the peak profiles are less amenable to analysis. Nevertheless, the higher resolution of conventional x-ray equipment is a very desirable feature, and efforts are being made to exploit this. Encouraging results have been obtained for several systems, such as $PbMo_6S_8$, one of a large group of compounds with superconducting properties. The advent of the NSLS is expected to lead to additional improvements in resolution which will open up the prospect of performing structural analysis at a level of complexity well beyond the present state of the art with polycrystalline materials.

SURFACE PHYSICS

The surface studies program is broadly based using many "state of the art" techniques to investigate the properties and interaction of various gases with solid surfaces. The major emphasis of the group is the development of a beam line at the NSLS for photoelectron spectroscopy on surfaces.

Electronic Properties of Surfaces and the Relationship to Hydrogen Dissociation

The mechanism by which molecules dissociate on surfaces is fundamental to questions of reactions on surfaces and how gases such as hydrogen enter bulk metals. It was discovered at Brookhaven that when palladium (Pd) is deposited on niobium (Nb) or tantalum (Ta) the first layer of Pd atoms go into the same sites that would be occupied by an additional layer of Nb. With subsequent layers, the Pd atoms start to transform to the structure of bulk Pd. Hence, we have a system where reactions can be studied on the same metal in two different crystal structures. Initial investigations have concentrated on the dissociation of hydrogen on these two Pd structures. Furthermore, the Nb provides a way of detecting when hydrogen goes through the Pd into the underlying Nb, since when this happens the resistance of the Nb increases. In the early stages, it was discovered that hydrogen cannot pass effectively through the first Pd layer which is in the Nb structure, but it very rapidly passes through the layer when the Pd transforms to its bulk structure. Various experiments show that when the hydrogen does not pass through the Pd layer the molecule does not dissociate, whereas when it does pass through the layer, essentially every molecule that impinges on the surface dissociates and then the atoms diffuse directly into the underlying Nb.

To understand this problem of what surface properties are necessary to dissociate molecules, photoelectron spectroscopy has been used to probe the electronic states in the two structures. By using both synchrotron radiation and a laboratory discharge lamp and analyzing the energy and angle of the photoemitted electrons from Pd for different wavelengths of light and crystal orientations, it has been possible to gain a fairly complete knowledge of the electronic structure of the two types of Pd. It was found that when the Pd is in the Nb structure, the Pd d-bands are below the level of the highest energy conduction band electrons (called the Fermi level). On the other hand, when the transformation to the structure of bulk Pd occurs, the d-electrons now add to the number of electrons at the Fermi level. Hence, there is at least circumstantial evidence that these additional electron states at the Fermi level are important for dissociation of the incoming molecules.

The Electronic Properties of Hydrogenated Amorphous Silicon

When hydrogen is combined with amorphous silicon (Si) the favorable electronic properties make it a viable candidate for low cost photovoltaic cells. An important problem in the understanding of this material is how the Si-H bonds affect the electronic structure, such as the width of the band gap and the distribution of electron states in this gap. By increasing the sample temperature, it was possible to observe how the peaks in the photoelectron spectra are associated with the different Si-H bonds and to identify the bonds which were most responsible for the changes in electronic structure between amorphous Si without hydrogen and the hydrogenated material. The largest changes in electronic structure occurred when single Si-H bonds were broken at a temperature of about 550°C.

Selected Publications (Solid State)

J. D. AXE. Incommensurate structures (Invited). *Proc. Conf. Royal Society on "Neutron Scattering in Biology, Chemistry, and Physics," September, 1979. Philos. Trans. Roy. Soc. London* **290**, 593-603 (1980).

J. L. BLACK AND V. J. EMERY. Critical properties of two-dimensional models. *Phys. Rev.* **B 23**, 429 (1981).

R. A. COWLEY, R. J. BIRGENEAU, AND G. SHIRANE. Excitations and phase transitions in random antiferromagnets. *Proc. NATO Advanced Study Institute on Strongly-fluctuating Condensed-matter Systems, Geilo, Norway, April, 1979*, T. Riste, Ed., Plenum, New York (1980) pp. 157-181.

D. E. COX AND A. W. SLEIGHT. The preparation and characterization of $Ba_3Te_2O_8$: A new oxide structure. *Acta Cryst.* **B35**, 1-10 (1979).

M. EL-BATANOUNY, M. STRONGIN, G. P. WILLIAMS, AND J. COLBERT. The relationship between electronic structure and hydrogen uptake kinetics. *Phys. Rev. Lett.* **46**, 269 (1981).

J. W. DAVENPORT. Infrared intensity and the CO metal bond. *Chem. Phys. Lett.* **77**, 45 (1981).

G. J. DIENES, D. O. WELCH, AND A. PASKIN. The self-consistent cell model equation of state for solids. *J. Phys. Chem. Solids* **41**, 1373-1381 (1980).

C. R. FINCHER, JR., S. M. SHAPIRO, A. C. PALUMBO, AND R. D. PARKS. Spin-wave evolution crossing from the ferromagnetic to spin-glass regime of Fe_xCr_{1-x}. *Phys. Rev. Lett.* **45**, 474-477 (1980).

Y. FUJII, O. SHIMOMURA, K. TAKEMURA, S. HOSHINO, AND S. MINOMURA. The application of a position-sensitive detector to high pressure x-ray diffraction using a diamond-anvil cell. *J. Appl. Cryst.* **13**, 284-289 (1980).

A. K. GHOSH AND M. STRONGIN. "Density of states of T_c of disordered A15 compounds," in *Superconductivity in d- and f-band Metals*, edited by H. Suhl and M. B. Maple. Academic Press, 1980.

J. A. GOLOVCHENKO, A. N. GOLAND, J. S. ROSNER, C. E. THORN, H. E. WEGNER, H. KNUDSEN, AND C. D. MOAK. Charge state dependence of channeled ion energy loss. *Phys. Rev.* **B** (in press).

J. B. HASTINGS. "EXAFS of dilute systems" in *EXAFS Spectroscopy: Techniques and Applications*, Plenum Press, New York (in press).

P. W. LEVY AND K. J. SWYLER. Radiation damage studies on natural and synthetic rock salt. *Workshop on Alternate Nuclear Waste Forms and Interactions in Geologic Media, Gatlinburg, TN, May 13-15, 1980.*

J. W. LYNN, G. SHIRANE, W. THOMLINSON, AND R. N. SHELTON. Competition between ferromagnetism and superconductivity in $HoMo_6S_8$. *Phys. Rev. Lett.* **46**, 368-371 (1981).

K. G. LYNN. Observation of the amorphous-to-crystalline surface transition in Al-Al_2O_3 using slow positrons. *Phys. Rev. Lett.* **44**, 1330-1333 (1980).

K. G. LYNN AND H. LUTZ. Studies of slow positrons in single crystal samples of Al and Al-Al_2O_3. *Phys. Rev.* **B 22**, 4143-4160 (1980).

D. E. MONCTON, G. SHIRANE, AND W. THOMLINSON. The development of magnetic order in superconducting systems (Invited). *Proc. Intern. Conf. Neutron Scattering and Magnetism, Julich, Germany, August, 1979.*

Z. OVADYAHU. Transition to zero vorticity in a 2-D superconductor. *Phys. Rev. Lett.* **45**, 375 (1980).

G. REITER. Have solitons been observed in $CsNiF_3$? *Phys. Rev. Lett.* **46**, 202-205 (1981).

G. SHIRANE. "Neutron diffraction and scattering," in *Encyclopedia of Physics*. R. G. Lerner and G. L. Trigg, Eds., (Addison-Wesley, Reading, MA, 1981) pp. 653-656.

R. J. SMITH. Photoemission studies of hydrogen chemisorption on niobium. *Phys. Rev.* **B 21**, 3131 (1980).

R. J. SMITH, G. P. WILLIAMS, J. COLBERT, M. SAGURTON, AND G. J. LAPEYRE. Electronic structure of the Nb(110) surface. *Phys. Rev.* **B 22**, 1584-1588 (1980).

M. STRONGIN, M. EL-BATANOUNY, AND M. PICK. The structure of Pd overlayers on Nb and Ta and the relationship to hydrogen uptake. *Phys. Rev.* **B 22**, 3126 (1980).

W. THOMLINSON, J. A. TARVIN, AND L. PASSELL. Excitations in few-atomic-layer adsorbed helium films: The two-dimensional roton. *Phys. Rev. Lett.* **44**, 266-269 (1980).

R. E. WATSON AND M. L. PERLMAN. Photoelectron spectroscopy of solids. *Phys. Scripta* **21**, 527-534 (1980).

R. W. YOUNGBLOOD AND J. D. AXE. Polarization fluctuations in ferroelectric models. *Phys. Rev.* **B 23**, 232-238 (1981).

R. YOUNGBLOOD, B. C. FRAZER, J. ECKERT, AND G. SHIRANE. Neutron scattering study of the pressure dependence of short-range order in CsD_2PO_4. *Phys. Rev.* **B 22**, 228-235 (1980).

In recent years the scope of accelerator-based atomic physics experiments has been greatly widened by the use of heavy ion beams from tandem accelerators. At Brookhaven it is now possible to produce beams of almost any element with energies from a few MeV to a few hundred MeV with the MP-Tandem Facility. However, in general, since ions of a particular charge state are produced by passing the beam through a stripping foil, it was not possible to produce ions of a given charge state at an arbitrary velocity. In many experiments measurements as a function of ion charge state at a fixed velocity, or as a function of velocity for a fixed charge state, are extremely important, but have been possible only over limited ranges of the parameters.

The BNL Tandem Facility can be used in an ingenious mode to greatly improve the range in which ion charge state and velocity can be treated as independent. This is accomplished by using the two tandems in a four-stage, acceleration-deceleration, mode. The injector tandem, MP-6, is run as a normal tandem, with positive terminal potential, to produce energetic positive ions. The second tandem, MP-7, is run with a negative terminal potential. The positive ions from MP-6 are thus given a third stage of acceleration to the terminal of MP-7 where they are passed through a gas or foil stripper and are stripped to a higher charge state. The fourth state is now a deceleration stage as the ions traverse the tube from the terminal of MP-7 back to ground potential. The method is extremely useful in producing low velocity beams of highly charged ions. It should be possible to produce essentially zero energy beams of fully stripped ions up to at least titanium with this technique.

We have employed this new breakthrough in ion beam technology in exploratory experiments with a sulfur beam. Sulfur was chosen for the initial work since intense beams can be easily produced, and it is comparatively easy to produce usable amounts of the highly charged ions, even if all the accelerator conditions are not optimized. The experimental equipment included electrostatic charge state analyzers before and after a differentially pumped gas cell viewed with a high resolution silicon x-ray detector. Measurements were made of the cross sections for electron capture by the beam from atoms of He, O_2, and Ar as a function of charge state at 20 MeV and as a function of energy from 6 to 20 MeV for q = 12^+, 13^+. The cross section production for K x-ray production was also measured at 20 MeV as a function of charge state for S-Ar and S-He collisions. The data obtained for the electron transfer excitation curve are shown in Fig. 1. There are several reasons why these measurements are of interest. From our standpoint, the main reason is the ability to probe the various channels involved in inner-shell vacancy production with a delicacy and precision not previously possible. The result of these and other experiments on the S-Ar system should give new and precise insights into the models, such as the molecular orbital model, which describe the complex ion-atom collision process.

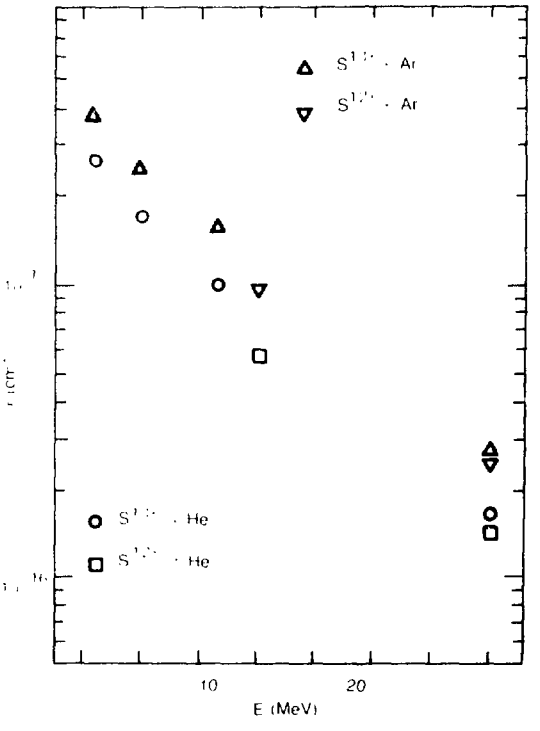

Figure 1. Total electron capture cross sections for $S^{12+,13+}$ for He and Ar targets as a function of ion energy.

Applied physics experiments are in progress in diverse fields with the main emphasis lying in the use of ion beams from the 3.5-MV Research Van de Graaff Accelerator for elemental analysis with high sensitivity and spatial resolution. A typical experiment which illustrates the utility and power of these techniques is the study of the migration of molybdenum in graphite at high temperatures.

The migration of fission fragments through graphite at elevated temperatures is of great interest to safety studies of high temperature gas reactors, which deal with hypothetical loss of coolant events with extremely high temperature excursions. The actual measurement of migration rates for fission fragments would be difficult because of the radioactivity, but equivalent information can be gained from use of stable isotopes in the medium mass region. The present work used Mo as representative of fission fragments.

For cases of very high temperatures and long heating times the Mo migrates over long distances, and ordinary chemical methods can be used to ascertain concentration gradients. For smaller distances this approach is no longer feasible, and recourse must be had to other methods. The use of the proton microprobe is ideal because of its excellent spatial resolution and high Mo detection sensitivity. Measurements were made on a variety of reactor grade graphite samples heated with Mo to temperatures from 1800 to 3100°C. The measured spatial distributions showed the presence of a pronounced microstructure probably due to agglomeration of Mo in the pores and along grain boundaries in the graphite. Diffusion coefficients derived from the data are much larger than for a simple bulk transport mechanism. For cases where comparison could be made, diffusion coefficients derived from the microprobe work were in good agreement with those found from chemical XRF determinations. Figure 2 shows results obtained for several scans of Mo concentrations around the central axis of a sample heated for two hours at 1800°C. The structure in the curves shows the existence of the Mo agglomerates. The sensitivity of the proton microprobe is much better than the electron microprobe, and only with the proton probe could these data have been obtained. Further experiments with heavier elements such as U or Th as well as the application of ion implantation and Rutherford backscattering techniques for very low temperature diffusion measurements will be of interest in the future.

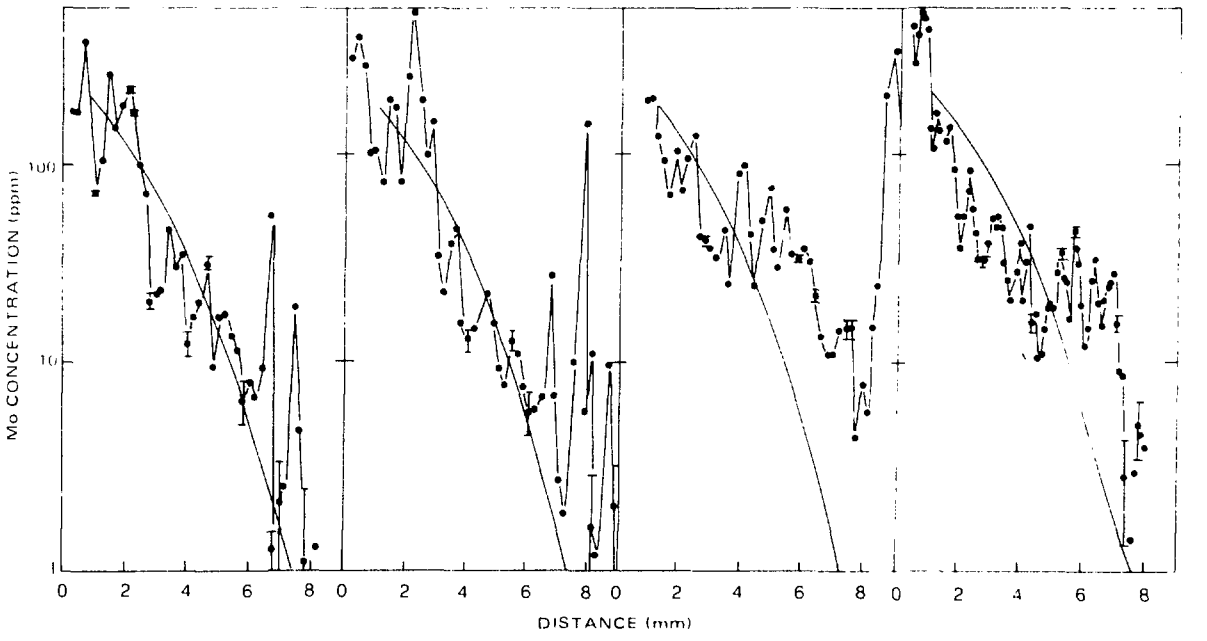

Figure 2. Four scans of the Mo distribution around the center axis of a sample heated for two hours at 1800°C. The solid line is a fit for a diffusion coefficient of 3.6×10^{-6} cm^2 sec.

Selected Publications

(Atomic and Applied Physics)

S. B. DOTY, K. W. JONES, H. W. KRANER, R. E. SHROY, AND A. L. HANSON. Proton microprobe analysis of zinc in skeletal tissues. *Nucl. Instrum. Methods* **181,** 159-164 (1981).

I. TSERRUYA, B. M. JOHNSON, AND K. W. JONES. Unexpected charge state dependence of K-x rays produced by S^{+q} and Ti^{+q} ions. *Phys. Rev. Lett.* **45,** 894-897 (1980).

R. SCHUCH, G. GAUKLER, G. NOLTE, K. W. JONES, AND B. M. JOHNSON. Impact-parameter dependence of 2 $p\pi$- and 1 $s\sigma$-molecular orbital x rays produced by Nb-Mo collisions at 143 MeV. *Phys. Rev.* **A 22,** 2513-2518 (1980).

B. M. JOHNSON, K. W. JONES, J. L. CECCHI, AND T. H. KRUSE. EUV spectra of Mo XIV to Mo XXIX. *Phys. Lett.* **78A,** 61 (1980).

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National Synchrotron Light Source

INTRODUCTION

The National Synchrotron Light Source (NSLS), under construction for the past two years, will be an extremely powerful source of visible and ultraviolet light and of "soft" and "hard" x-rays. As a source of light, it will be more intense than a laser; as an x-ray source, it will be 10 to 100 times more powerful than standard x-ray tubes. When completed, hundreds of researchers can use the machine simultaneously.

Although the machine looks like the accelerators used in high energy physics research, it will be used to study atoms and their interactions rather than nuclei. Innumerable problems exist in the field of the basic properties of matter: in the arrangement of atoms in crystals, in the behavior of surfaces, in liquid behavior, in biological samples, and so forth. Not only will the machine be used by researchers from universities and government laboratories, but also there is great interest in it on the part of industry. For example, IBM wants to learn how x-rays can be used in the fabrication of micro-circuits, and Exxon wants to study catalysis. At this writing, it seems the demand for beam time will not be met even with 24-hour operation.

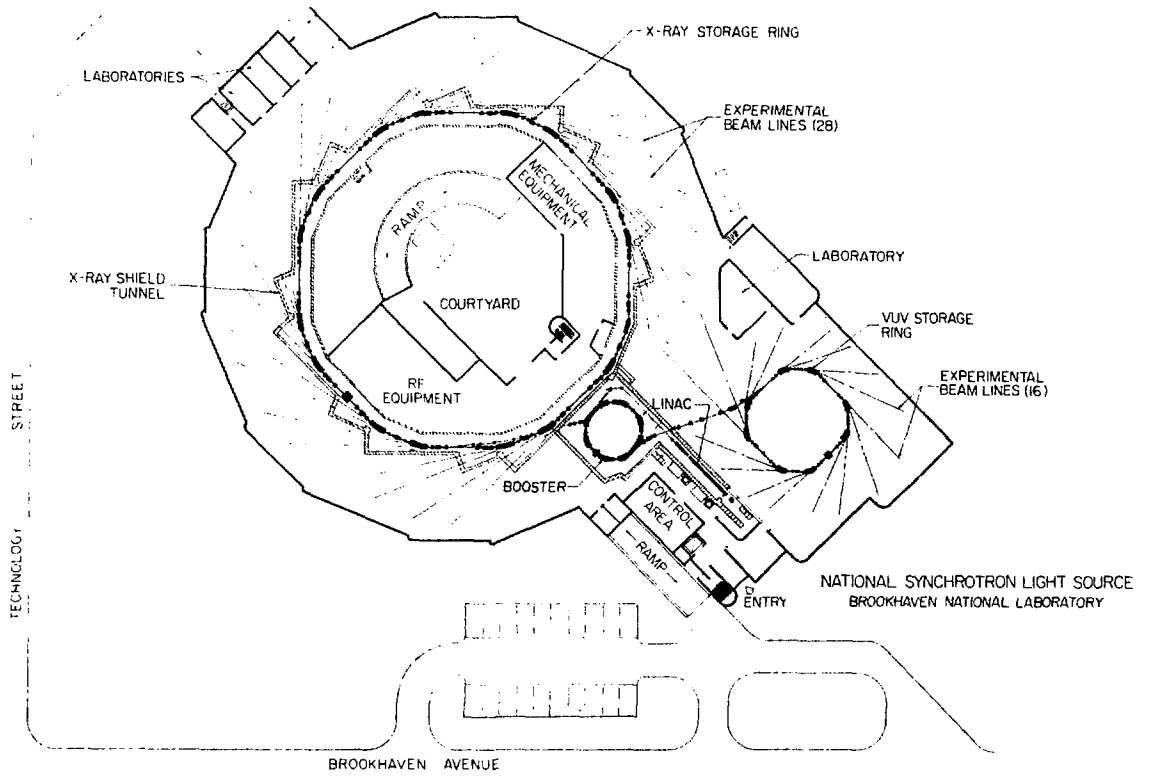

Figure 1. Plan view of the NSLS. The large ring is the x-ray source. The next smaller ring will provide vacuum ultraviolet (VUV) and visible light, and the smallest ring (Booster) is a synchrotron that will serve as injection for both storage rings. The booster is fed by the small Linac. A total of 44 beam lines (28 x-ray and 16 VUV) is indicated.

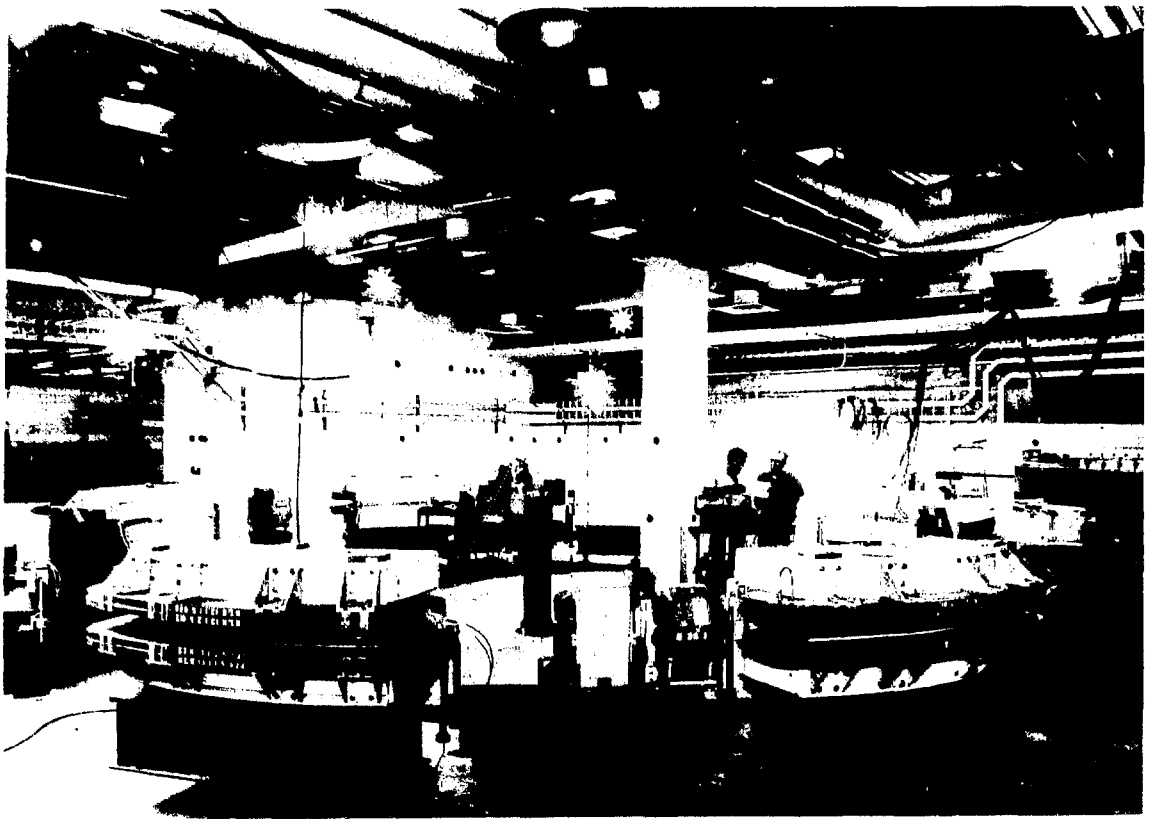

Figure 2. The Booster Synchrotron in process of assembly.

CONSTRUCTION PROGRESS

The building (725), for which ground was broken on September 28, 1978, is substantially complete. The NSLS staff is scheduled to move in January 1981, and final assembly of the machine components should proceed swiftly. Figure 1 is a sketch of the machine layout. Electrons start in the Linear Accelerator (LINAC) and are accelerated to 70 MeV. At this energy, they are injected into the Booster synchrotron where their energy is increased by a factor 10. The 700 MeV electrons are then injected into one or the other of the storage rings as needed. In the x-ray ring the electrons are further accelerated to 2.5 GeV; in the Vacuum Ultraviolet (VUV) ring, their energy is constant, with only enough rf supplied to replace the energy lost by radiation. In each ring, the stored electron beam will be about 1/2 ampere.

The Linear Accelerator, Booster (Fig. 2), and VUV ring (Fig. 3) installations are virtually complete. Beam tests have been carried out on the Linac and Booster using the central control computer which was still located in Building 925.

Beam tests on the VUV ring and acceleration in the Booster ring await completion of the process water systems which should occur soon. Survey work is already under way in the x-ray ring tunnel, and installation of the magnetic components, which are currently being fabricated and tested in Building 919, will follow. Radiofrequency systems for the Booster and VUV rings have been operated at design levels and fabrication of the x-ray storage ring rf system has started. Vacuum and beam diagnostic hardware for the x-ray ring is also well advanced.

BEAM LINES AND EXPERIMENTAL EQUIPMENT

In parallel with installation and testing of storage ring components, work is well ad-

vanced on experimental equipment. Up to four beam lines are expected to be placed on the VUV storage ring by mid-1981 and three assembled on the x-ray ring by the year's end. An even larger number of beamlines are presently under development by outside groups. These come from corporate, university, and national laboratory organizations that have formed a partnership with Brookhaven for utilization of the light source. They are designated "Participating Research Teams" and will be installing their beamline hardware on a similar timescale to the NSLS.

These is great variety in the instrumentation used in harnessing synchrotron radiation for research. It is necessary to design special instruments to take best advantage of the intensity, wide spectral coverage, collimation, polarization, and vacuum cleanliness of the source. The investment in hardware for experiments is high and is expected to eventually overtake the 24 million dollars spent on the Light Source itself. An example of an extreme UV/soft x-ray monochromator is shown in Fig. 4. This ultrahigh-vacuum, plane-grating instrument will cover the range 20-1000Å with a resolving power on the order of 5000. The figure shows the internal mechanism mounted on a jig for acceptance trials.

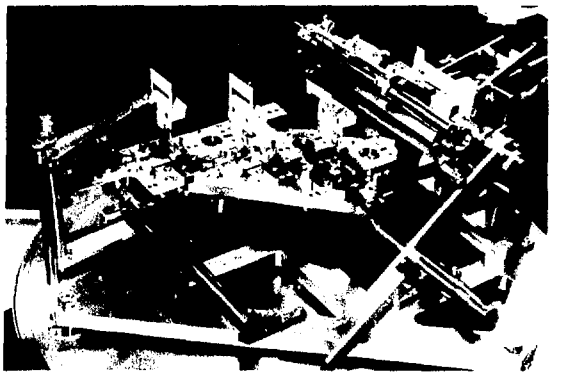

Figure 4. Mechanism for plane grating monochromator as supplied by manufacturer. The four rectangular mounts with circular holes just above the center will carry paraboloidal focusing mirrors, each designed to work at a different grazing angle. The mechanism above and to the right will carry two interchangeable diffraction gratings. At the upper right is the mount for a collimating mirror. The diagonal arm at the lower right is driven vertically thereby rotating the diffraction grating to scan the wavelength range.

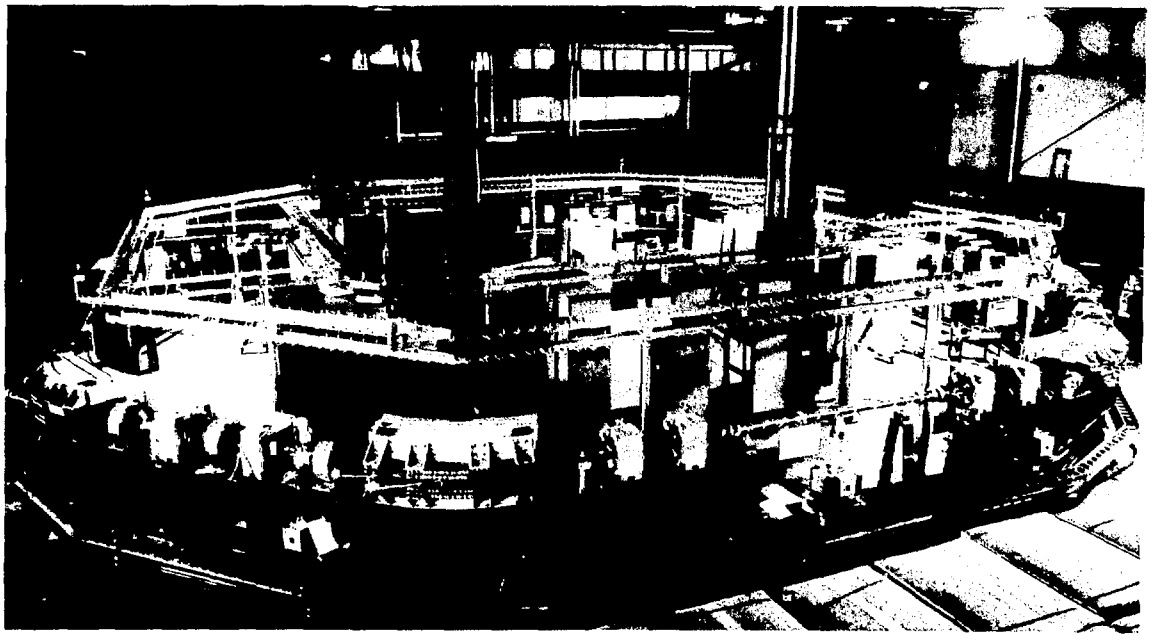

Figure 3. The VUV ring nearly complete. Note that this is not really a ring but has 8 straight sections, where the beam is focused, rf acceleration is applied, and vacuum pumps are attached, and 8 curved sections where the beam is bent by magnets, giving rise to the synchrotron radiation. Two beam ports are provided at each magnet.

NATIONAL SYNCHROTRON LIGHT SOURCE

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Chemistry Department

INTRODUCTION

Research activities in the Chemistry Department encompass a wide spectrum of topics, ranging from the study of organometallic catalysts to the investigation of nuclear processes occurring in the sun. Although many of the research programs are similar to those carried out in universities and other research institutions, others require facilities unique to Brookhaven, such as the High Flux Beam Reactor or various particle accelerators. To this list will soon be added the National Synchrotron Light Source. A significant fraction of the work described below represents research carried out in collaboration with colleagues within the Chemistry Department and other BNL Departments, or with scientists from universities and industry.

STRUCTURAL CHEMISTRY

Single Crystal X-Ray and Neutron Diffraction

At BNL, the powerful techniques of single-crystal X-ray and neutron diffraction analysis are used in structural studies of a wide variety of novel and interesting systems. Recent investigations have been concerned with transition-metal cluster compounds, metal-carbene complexes, and compounds with low melting points, among others. In work on the nitrogen oxides, NO_2 and N_2O_4, techniques were developed to grow large crystals directly by cooling from the gas phase while monitoring the crystallization process in a neutron beam at the High Flux Beam Reactor. The structure of N_2O_4 (Fig. 1) is noteworthy because of the exceptionally long N-N bond, weakened by non-bonded electron-pair repulsions.[1] Recent theoretical calculations performed here at Brookhaven are in agreement with the experimental N-N distance of 1.76 Å. The crystal-growing technique appears to be of general utility and should make possible studies of a number of simple molecules that exist as gases at room temperature, as well as the investigation of crystals held together by weak intermolecular forces.

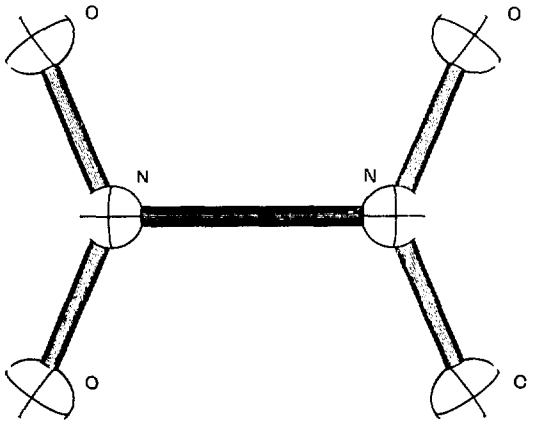


Figure 1. The structure of dinitrogen tetroxide.

In late 1981, the X-ray crystallography beam line planned for the National Synchrotron Light Source (NSLS) is scheduled to become operational. It will be possible to tune the intense beam from the synchrotron to obtain any desired X-ray wavelength over a wide range, thus allowing a number of new types of experiments to be performed. Among the studies planned for the initial period are structure analyses of complicated systems such as zeolites and peptides, and studies of electronic charge-densities in molecular solids. Together with the existing neutron diffraction instruments at HFBR, the NSLS will give BNL a unique combination of facilities for research in structural chemistry.

EXAFS Studies of Ions in Solution

Extended X-ray absorption fine structure (EXAFS) refers to the oscillation of the X-ray absorption coefficient of an element with increasing photon energy at energies above a characteristic threshold. This phenomenon arises from the interference of the waves of the outgoing and backscattered photoelectrons. It thus depends upon the nature and distance of the scattering atoms surrounding the atom absorbing the photons. EXAFS measurements

made at Stanford Synchrotron Radiation Laboratory have been employed to study the structures and dynamic behavior of transition metal ions in aqueous solution. Of particular interest in the present study are the structural parameters of the complex ions in the classic electron exchange reaction:

$$[Fe(H_2O)_6]^{2+} + [Fe(H_2O)_6]^{3+} \rightleftharpoons$$

$$[Fe(H_2O)_6]^{3+} + [Fe(H_2O)_6]^{2+} \qquad (1)$$

Here the reactants and products are chemically identical. According to theory, the coordination shells of the two reactants must attain identical configurations in the transition state for the reaction. Thus the difference between the mean Fe-O radii of $Fe(H_2O)_6^{2+}$ and $Fe(H_2O)_6^{3+}$ in solution, $r_2 - r_3$, is relevant to the rate constant for Eq. (1). Until these EXAFS solution results were obtained, the radius data available were for solids; in the solid state the $Fe^{II}-OH_2$ distance varies from 2.12 to 2.15 Å, depending upon lattice anion. EXAFS with synchrotron radiation, however, can be used conveniently to measure r_2 and r_3 for the ions in solution under conditions similar to those in which the exchange reaction occurs. The X-ray absorption spectrum of $Fe(H_2O)_6^{2+}$ and spectra related to data analysis are given in Fig. 2. The r_2 and r_3 values derived are 2.095 and 1.990 Å, respectively, at room temperature.[2] From these data, we obtain the radius in the activated complex $r^{\ddagger}$ = 2.030 Å and the free energy of activation $\Delta G^{\ddagger}$ = 14.7 kcal mole^{-1}; the latter is in reasonable agreement with experiment (16.6 kcal mole^{-1}). This rather large $\Delta G^{\ddagger}$, which corresponds to a slow reaction rate, may be rationalized qualitatively if one considers the large displacements required for the reactants to reach the activated state ($r_2 - r^{\ddagger}$ = 0.065 Å and $r^{\ddagger} - r_3$ = 0.040 Å for $Fe(H_2O)_6^{2+}$ and $Fe(H_2O)_6^{3+}$, respectively) in comparison with the relative small amplitudes of displacement during the totally symmetric stretching vibration of the complexes. The root mean square amplitudes, σ_{sym}, are 0.0233 and 0.0194 Å for $Fe(H_2O)_6^{2+}$ and $Fe(H_2O)_6^{3+}$, respectively.

THEORETICAL CHEMISTRY

Simple quantum chemical concepts and *ab initio* calculations have shed considerable light on the electronic structure of silica polymorphs (e.g., quartz) and the factors which control various pertinent geometrical features. Careful

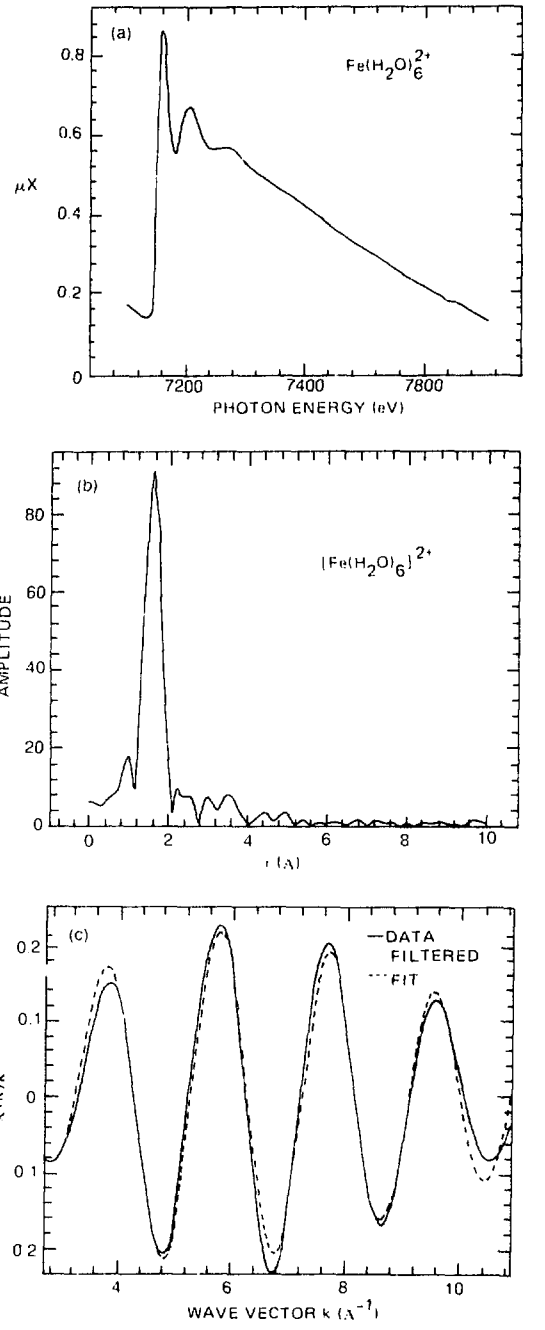


Figure 2. (a) X-ray absorption spectrum of $Fe(H_2O)_6^{2+}$, (b) Fourier transform of $\chi(k)k^3$, and (c) the filtered data and the best nonlinear least-squares fit for $Fe(H_2O)_6^{2+}$.

crystallographic studies reveal that the SiOSi bond angle (θ) covers a very broad range (120°-180°), depending on the local environment. Furthermore, the associated SiO bond length (r) is observed both from experimental data and from the present *ab initio* calculations to vary monotonically with respect to θ *via* the relationship:

$$r - r_0 = A/(1-\cos\theta),$$

where r_0 is the appropriate reference value and A is a constant. This bond length-bond angle relation is precisely what would be expected on the basis of simple hybrid atomic orbital concepts which predict that, as the angle (θ) between two equivalent s-p hybrid orbitals increases, the "fractional s-character" of the hybrids increases, and hence also, their bonding strength, thus leading to shorter bonds.

The inferred importance of oxygen orbital hybridization may appear somewhat surprising, since recent band structure calculations, which focused on photoemission spectra rather than energetics of geometrical distortion, have suggested that the oxygen 2s electron could be relegated to a relatively "inert" core. Accordingly, additional *ab initio* calculations were carried out, which allowed the electronic wavefunction of the disiloxyl group (Si⁄O⁄Si) to be analyzed explicitly in terms of valence orbital hybridization (this is not routinely done in conventional electronic structure calculations). These detailed calculations[3] fully confirm the qualitative inference based simply on the bond length-bond angle variation, as described above, and demonstrate that the atomic orbital character of the SiO bond is strongly dependent on the angular geometry of the divalent oxygen atom. Thus quartz and related species, although primarily associated with the element "silicon", have been shown to reveal a rich electronic as well as geometric structural diversity of the other constituent atom—i.e., oxygen.

LASER INDUCED PROCESSES IN THE GAS PHASE

Energy transfer in vibrationally excited molecules has been shown by a variety of techniques to involve several different types of relaxation pathways. Recently one of these pathways, near resonant vibration-to-vibration energy transfer, has been studied under single collision conditions subsequent to excitation with an intense infrared (IR) laser. A molecular beam of the molecule propynal, H—C≡C—CHO is excited with a CO_2 laser. Excitation of the ν_6 mode, C—C stretch, produces a distribution of molecules having energies ranging from 1 hν (energy of one photon, 951 cm^{-1}) to nhν. This distribution produced by the CO_2 laser alone is examined spectroscopically with a dye laser. Then collisions with other molecules are introduced one at a time and the resulting changes in the distribution are probed.

These experiments[4] have confirmed previous observations that the fastest relaxation process involves only the mode that is initially excited. However, several unexpected results have been obtained. Collisions do not equilibrate ν_6, the excited mode, and ν_{10}, a nondriven mode differing by only 40 cm^{-1} in energy from ν_6. This is contrary to theoretical predictions. Although the fastest energy transfer pathway involves the excited mode ν_6, quantum number changes $\Delta v > 1$ occur with the same rate as $\Delta v = 1$ in this mode. The latter has a rate constant much greater than gas kinetic. These observations suggest that energy transfer in highly excited polyatomic molecules occurs by additional pathways that normally are not observed either at lower excitation energies or in diatomics.

A research area that continues to be of great interest is infrared multiphoton dissociation (IRMPD) — the absorption of many infrared photons by a molecule and subsequent unimolecular dissociation. This type of reaction typically is induced by pulsed radiation from a CO_2 laser, and a convenient method for following the reaction is the observation of infrared chemiluminescence from either primary or secondary reaction products. As developed in our laboratory, an appropriate infrared detector is used to observe emission from hydrogen halides formed in the reactions

$$RCH_2CH_2X + nh\nu \rightarrow RCH{=}CH_2 + HX^{\ddagger} \quad (2)$$

or

$$RX + nh\nu \rightarrow R + X \quad (3)$$

$$X + AH \rightarrow A + HX^{\dagger},$$

where the dagger indicates vibrational excita-

tion. The second of these methods was recently used to study the IRMPD of the molecule CF_3Cl, with HBr as the hydrogen donor.[5] The unexpected result was that both $HF^{\dagger}$ and $HCl^{\dagger}$ were observed, in a ratio of about 1:3. This could result from vibrational excitation of CF_3Cl, leading to competitive eliminations of either F or Cl atoms, i.e.,

$$CF_3Cl^{\dagger} \rightarrow CF_3 + Cl \qquad (4a)$$

$$\rightarrow CF_2Cl + F \qquad (4b)$$

However, the critical energy for reaction (4a) is almost 40 kcal/mole below that for reaction (4b), and statistical reaction theory indicates that at the energy threshold for reaction (4b) the rate of (4a) is larger by one million. An alternative explanation for the appearance of F atoms is based on a secondary IRMPD of the CF_3 radical:

$$CF_3 + m h\nu \rightarrow CF_2 + F \qquad (5)$$

Confirmation of this was obtained by a search

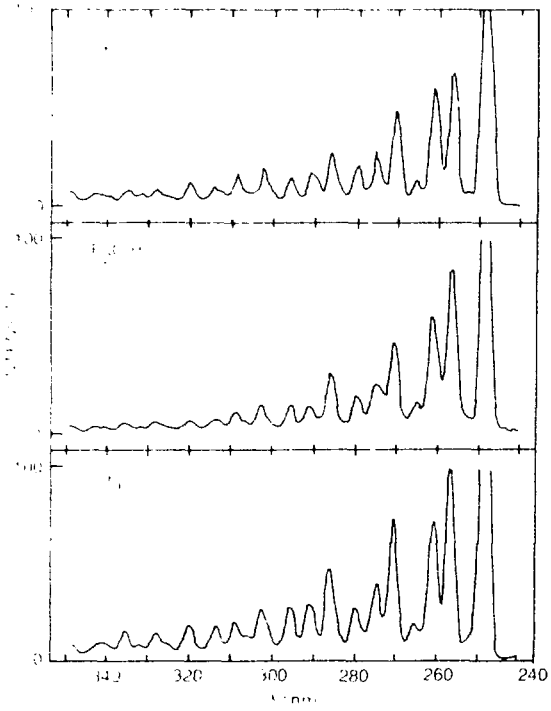


Figure 3. Laser-induced fluorescence signals. For each trace, P_{CF_3Cl} = 15.00 Torr, $P_{(CO_2)}$ = 15.25 Torr. CO_2 laser conditions were as follows: CF_3Cl R(40) line at 1090.03 cm^{-1}, fluence = 100 J/cm^2; CF_2HCl R(26) line at 1082.30 cm^{-1}, fluence = 40 J/cm^2; C_2F_6 R(36) line at 1087.95 cm^{-1}, fluence = 83 J/cm^2.

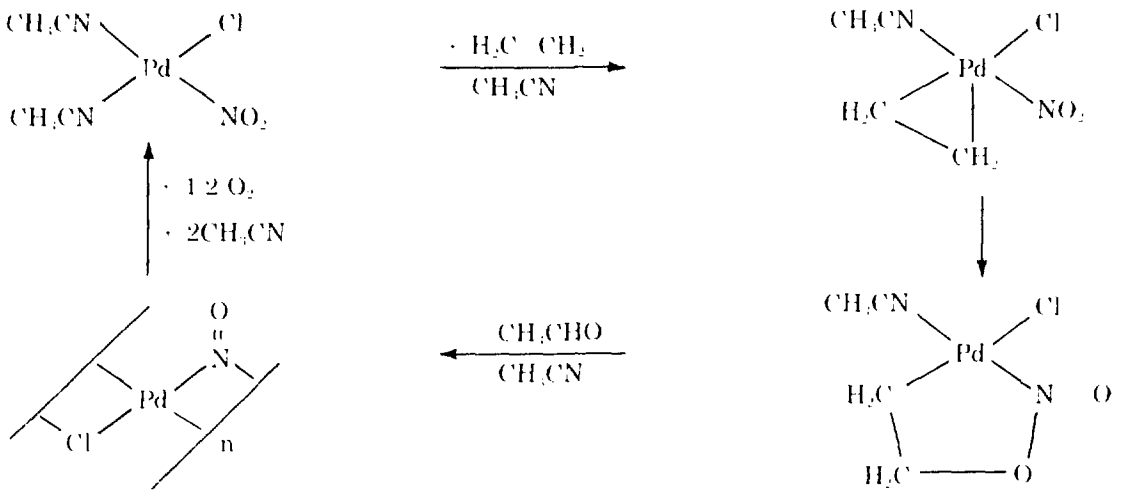
for difluorocarbene (CF_2), using laser-induced fluorescence as the analytical tool. Difluorocarbene is known to fluoresce strongly when excited at ~250 nm, a region accessible to a KrF excimer laser, which was pulsed ~0.5 μsec after the CO_2 laser pulse. The fluorescence spectrum obtained under these conditions is shown in the upper panel of Fig. 3. It is obviously the same as that of the center panel, obtained when CF_2HCl (a molecule previously shown to dissociate to CF_2 and HCl) is subjected to similar experimental conditions. To demonstrate that the IRMPD of the CF_3 radical is not unique to this reaction system, similar experiments were carried out with C_2F_6, which had previously been shown to yield large amounts of CF_3 radicals. Again, laser-induced fluorescence indicated the production of CF_2.

These experiments, and similar observations in the case of CF_3Br, SF_5Cl, and SF_6, indicate that IRMPD of primary products is not uncommon, and that attempts to determine mechanism by measuring yields of stable products may be misleading.

ORGANOMETALLIC CHEMISTRY AND HOMOGENEOUS CATALYSIS

A new project in the Chemistry Department is devoted to the study of organometallic compounds (molecules containing metal-carbon bonds). These complexes have important applications as homogeneous catalysts. Catalysts are species which are not consumed but which allow chemical reactions to occur more rapidly, at milder temperatures and pressures, and with greater selectivities. The chemical industry makes extensive use of catalysts to increase process efficiencies and to conserve energy and natural resources. At BNL, a search is underway for new olefin oxidation catalysts. Oxidation of olefins such as ethylene and propylene is carried out commercially in large volumes to prepare solvents (acetone, methylethyl ketone) and valuable chemical intermediates (ethylene oxide, acetaldehyde) which ultimately find their way into antifreezes, textiles, detergents, and plastics. A new type of olefin oxidation catalyst has been found at BNL which makes use of a transition metal nitro-nitrosyl redox couple.[6] As is shown in Scheme I, a metal nitro complex ($M\text{-}NO_2$) coordinates an olefin (ethylene, $H_2C=CH_2$) to the metal, forming an organ-

Scheme I

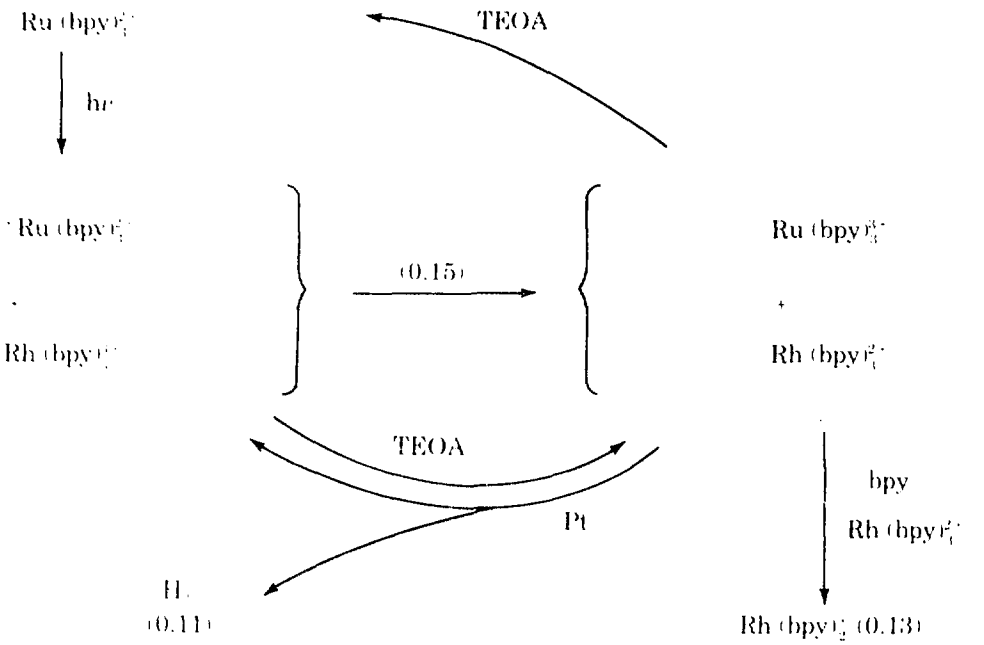


ometallic complex containing metal-carbon bonds. The nitro group then transfers an oxygen atom to the olefin to give oxidized olefin (acetaldehyde, CH_3CHO) and a reduced metal nitrosyl (M-NO). The metal nitrosyl is then oxidized by atmospheric oxygen, regenerating the starting metal nitro complex. While the metal nitro complex takes part in the reaction, it is not consumed in the overall reaction which converts air and ethylene into acetaldehyde. Detailed studies of reaction intermediates and mechanisms are providing information which will lead to the development of better catalysts and catalysts which direct the olefin oxidation towards different products such as ethylene oxide.

INORGANIC REACTION MECHANISMS

Electron-transfer (oxidation-reduction) reactions are the most useful type of photochemical reaction for solar energy conversion and storage. Certain metal complexes absorb light strongly in the visible region and readily exchange electrons with suitable substrates and so are useful mediators for the collection and storage of solar energy. Thus the photo-induced reactions of 2,2′-bipyridine (bpy) complexes of transition metals (especially ruthenium) are under investigation with the focus being the mediated photodecomposition of water into hydrogen and oxygen. This research effort has recently[7,8] permitted the elucidation of the detailed mechanism of a rather complex system which effects the photoreduction of water. In this system hydrogen, but not oxygen, is produced; the reducing equivalents are provided by the organic molecule triethanolamine. The irradiation of aqueous solutions containing $Ru(bpy)_3^{2+}$, $Rh(bpy)_3^{3+}$, and triethanolamine (TEOA) with visible light yields a rhodium(I) complex, but, when platinum is present, hydrogen is formed instead. A detailed mechanistic scheme, Scheme II (in which quantum yields—the number of molecules of product per photon absorbed—are given in parentheses), has been deduced from the results of pulse radiolysis and continuous and flash photolysis experiments: light absorption by $Ru(bpy)_3^{2+}$ gives the excited state $^*Ru(bpy)_3^{2+}$ which is oxidized by $Rh(bpy)_3^{3+}$ yielding $Ru(bpy)_3^{3+}$ and $Rh(bpy)_3^{2+}$. Back reaction of $Ru(bpy)_3^{3+}$ with $Rh(bpy)_3^{2+}$ is prevented by the reduction of $Ru(bpy)_3^{3+}$ by TEOA. The oxidized TEOA radical so generated undergoes a TEOA promoted rearrangement to a reducing radical. The latter reduces $Rh(bpy)_3^{3+}$ so that the $Rh(bpy)_3^{2+}$ yield is doubled. Rate determining loss of bpy from $Rh(bpy)_3^{2+}$ is followed by rapid reduction of $Rh(bpy)_2^{2+}$ by $Rh(bpy)_3^{2+}$ giving $Rh(bpy)_3^{3+}$ and Rh(I). In the presence of platinum, H_2 is formed at the expense of Rh(I); catalyzed reaction of

Scheme II



Rh(II) with water occurs before disproportionation to Rh(I) can take place. Because the homogeneous and heterogeneous dark reactions are so very efficient, the H_2 quantum yield in this system is limited only by the cage escape of the primary products. The efficiency is further enhanced by the TEOA radical rearrangement which converts an oxidizing species into a strong reductant thus promoting the accumulation of the crucial Rh(II) intermediate.

PICOSECOND SPECTROSCOPIC STUDIES OF INTRAMOLECULAR ELECTRON TRANSFER

The oxidation of iron (II) cytochrome c (Fe(II) cyt-c) is one of the earliest studied light-driven electron transfers (ETs) associated with the primary events of bacterial photosynthesis.[9-11] In *Chromatium vinosum* the reaction takes 1 μsec at room temperature and completes an ET cycle that begins with the oxidation of a bacteriochlorophyll dimer, $(BChl)_2$.[12-14] Several theoretical descriptions of this ET have been given[11,15] and an experimental estimate of the minimum edge-to-edge separation of the electron donor and acceptor of 15 ± 3 Å has been made.[16]

Recently we have studied the dynamical properties of the diporphyrin Zn-Fe(III)Cl (shown in Fig. 4) following photoexcitation to provide additional data for modelling the naturally occurring cyt-c oxidation.[17]

When Zn-Fe(III)Cl is photoexcited new photochemical processes not seen for either of the isolated subunits are found. The absorption

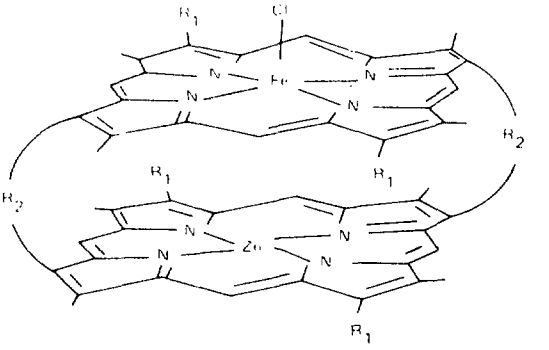


Figure 4. Structural drawing of the Zn-Fe(III)Cl diporphyrin. The side chains, R_1, are n-octyl groups and the linking chain, R_2, is

$$R_2 = -CH_2-C(=O)-N(\text{n-butyl})-CH_2-CH_2-$$

cross-section of the rapidly formed ($\tau \lesssim 10$ psec) photoproduct is at least twice as large as those of the excited states of Fe(III)Cl octaethylporphine (Fe(III)ClOEP) and its broad visible absorption is consistent with the formation of a Zn–porphyrin cation ($Zn P^{+}$). Figure 5 shows a plot of the decay of this photoproduct's absorption at 600 nm in two solvents, tetrahydrofuran (THF) and pyridine. The decay is not first order in either one and has initial half-lives of 25 and 200 psec, respectively, in THF and pyridine.

These results are consistent with the following ET reaction

$$Zn\text{-}Fe(III)Cl \rightarrow |Zn^{+}\text{-}Fe(II)|Cl \qquad (6)$$

In this case the non-exponential decay shown in Fig. 5 is likely to be due to the dissociation of the Cl^{-} ion from its axial position on Fe(II) during the reverse ET

$$|Zn^{+}\text{-}Fe(II)|Cl \rightarrow Cl^{-} + Zn\text{-}Fe(III)^{+} \qquad (7)$$

The reassociation of Cl^{-} to form Zn-Fe(III)Cl may take several hundred picoseconds.

The reverse ET in Reaction 7 is analogous to the reduction of $(BChl)_2^{+}$ by Fe(II)cyt-c in photosynthetic bacteria.[9-13] A major difference contributing to the ~ 4 orders of magnitude difference in rates for these two ETs is the distance of separation of the electron donors and acceptors

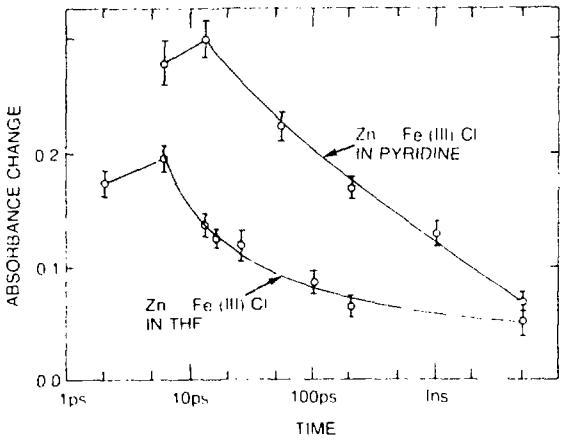


Figure 5. Plots of the change in absorbance for Zn-Fe(III)Cl in tetrahydrofuran and pyridine at 600 nm following excitation at 527 nm with a 6 psec laser pulse. The samples' concentrations were, respectively, 1.8×10^{-4} M and 3.3×10^{-4} M.

in the two cases. Cyt-c and $(BChl)_2$ are about 15 ± 3 Å apart[16] while the porphyrin subunits in Zn-Fe(III)Cl are 4—5 Å apart.[18] These reaction rates can be compared by asking to what distance would the porphyrin subunits in Zn-Fe(III)Cl have to be separated to slow the reverse ET by four orders of magnitude. Using a theoretical estimate[15] of the distance dependence of the electronic coupling which controls ET reactions, the required separation is calculated to be 11—12 Å. Surprisingly this answer does not differ significantly from the experimental estimate[16] of 15 ± 3 Å for the cyt-c to $(BChl)_2$ separation. That the rate of the reverse ET in this model system appears to correlate with a well studied, naturally occurring ET is encouraging. Future studies are aimed at exposing more of the details of this important class of chemical reactions.

NUCLEAR CHEMISTRY

Investigation of the reactions between energetic projectiles and complex nuclei is a continuing program in the Chemistry Department. This work entails both experimental studies of cross sections and momenta of target fragments as well as the development of theoretical models which are useful for understanding the mechanisms leading to the complex mixture of products.

As an energetic projectile approaches a nucleus, it sees the target foreshortened as a consequence of the Lorentz contraction. Apparent geometries for 0-, 2-, and 10-GeV protons incident on ^{197}Au are shown in Fig. 6(a). At sufficiently high energies, the interactions of the proton with nucleons in the cross-hatched interaction volume may be collective in nature, and they can be treated as a single interaction with an effective target having a mass Δm. From such a collective tube model (CTM) and from the conservation laws, it follows that the forward momentum, $q_{\parallel}$, transferred to the spectator parts of the target can be related to the energy transferred, ΔE, and to the projectile velocity, β, and total energy, E, by the relationship

$$\beta q_{\parallel} = \Delta E + \Delta E \Delta m / E.$$

Experimental data (obtained elsewhere) for the production of ^{149}Tb from ^{197}Au by high-ener-

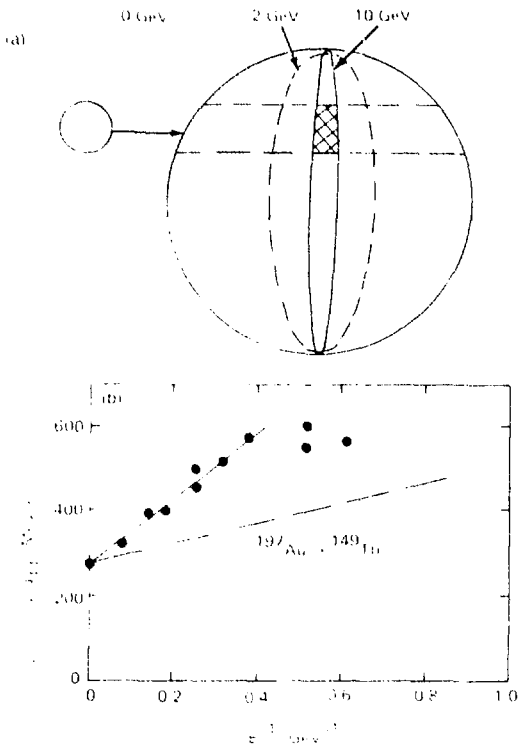


Figure 6. (a) Schematic diagram showing effects of Lorentz contraction on a ^{197}Au target as seen by a proton of 0-, 2-, and 10-GeV kinetic energy. (b) Dependence of reduced momentum, $\beta q_{\parallel}$, on reciprocal of the bombarding particle's total energy for ^{149}Tb production from ^{197}Au targets. The solid line is a least squares fit to the points for $E^{-1} < 0.4$. The dashed curve shows the dependence predicted by an older model.

gy protons are presented in the form of a plot of reduced momentum, βq_0 , vs E^{-1} in Fig. 6(b). Results at high energies ($E^{-1} < 0.4$) are consistent with the linear dependence predicted by the above equation and yield a value of $\Delta m = 3.1 \pm 0.4$ nucleons. Deviations which appear at $E^{-1} > 0.4$ are probably a consequence of the simplifying assumptions of the model. The dashed line in Fig. 6(b) shows that an existing model, which has frequently been used for the analysis of target fragmentation data, cannot account for the changes of over a factor two at high bombarding energies. This older model appears functionally as a special case of the CTM for which $\Delta m = 1$. It is thought that the more general equation will serve as a new and useful framework for systematizing and interpreting a wide variety of experimental data including those from studies using energetic heavy-ion projectiles.[19]

THE BROOKHAVEN SOLAR NEUTRINO PROGRAM

The nuclear reactions powering main sequence (hydrogen-burning) stars such as the sun are thought to be known and the detailed structures of such stars are thought to be well understood.[20] The Brookhaven solar neutrino program is a long-term attempt to obtain experimental confirmation about the nuclear processes in the energy-generating part of the sun by observing the neutrinos emitted in these processes. A complete measurement of the fluxes and energies of all of the neutrinos emitted by the sun would allow us to understand exactly the energy-producing processes in the sun. During the last eleven years an experiment has been operating which is sensitive predominantly to the high energy neutrinos from the sun. This experiment is based on the capture of neutrinos by the stable ^{37}Cl to produce radioactive ^{37}Ar:

$$^{37}\mathrm{Cl} + \nu \underset{\text{decay}}{\overset{\text{capture}}{\rightleftharpoons}} {}^{37}\mathrm{Ar} + \mathrm{e}$$

{Energy threshold = 0.816 MeV
Half-life for decay = 35 days

Because most of the neutrinos from the sun have energies below the energy threshold for this reaction, it is sensitive to only a small fraction of the solar neutrino spectrum.

The results provided by this experiment are about a factor three lower than those predicted by the most reasonable theoretical models of the sun. These low results can be accounted for by some process which lowers the internal temperatures of the sun. Another suggestion is that we do not understand the basic properties of neutrinos. Perhaps the neutrinos oscillate to another non-reactive type of neutrino on their journey from the sun to the earth. The possiblity of neutrino oscillations is presently being considered very seriously. Some evidence now exists that electron anti-neutrinos from a reactor may oscillate on a distance scale of a few meters.

Although the combined results of the chlorine experiment can be interpreted as being

caused by neutrino oscillations, this does not constitute strong evidence for neutrino oscillations because other explanations are possible. However, a second solar neutrino experiment could provide an answer to the questions of possible neutrino oscillations and of why the result of the chlorine experiment is low. The best radiochemical experiment for this purpose uses ^{71}Ga as target and produces radioactive ^{71}Ge according to the reaction:

$$^{71}\text{Ga} + \nu \underset{\text{decay}}{\overset{\text{capture}}{\rightleftharpoons}} {}^{71}\text{Ge} + e$$

Energy threshold = 0.235 MeV
Half-life for decay = 11.8 days

The threshold for this reaction is low enough that a major fraction of the neutrinos from the sun are capable of producing this reaction. Performing a gallium solar neutrino experiment has been for several years a major objective of a collaboration consisting of the Max Planck Institute for Nuclear Physics at Heidelberg, the Weizmann Institute, the University of Pennsylvania, the Institute for Advanced Study, and Brookhaven National Laboratory.

During 1980 at Brookhaven a pilot experiment (Fig. 7) was set up containing 1.3 tons of Ga as an aqueous solution of $GaCl_3$ acidified with hydrochloric acid.[21] The product of the neutrino capture, ^{71}Ge, is simply removed as gaseous $GeCl_4$ by passing an inert gas through the solution. After conversion to a gas suitable for counting, the decays of ^{71}Ge are counted in a proportional counter. This pilot experiment has demonstrated that ^{71}Ge can be removed from the solution and placed in a small counter with nearly 100% efficiency. Studies of all possible background processes show that they can be controlled sufficiently to observe a clear solar neutrino signal. The technical feasibility of a full scale solar neutrino experiment using 50 tons of gallium has been demonstrated.

Although the capture cross-section of neutrinos by ^{71}Ga has been accurately calculated, it is very desirable to measure this cross-section experimentally. This measurement could be accomplished using a prepared source of neutrinos of known energy and known intensity. A possible source is provided by neutrinos from the decay of ^{51}Cr, which can be prepared in a high flux nuclear reactor. With such a source, it is relatively simple to also look for neutrino oscillations at distances of a few meters from the source.

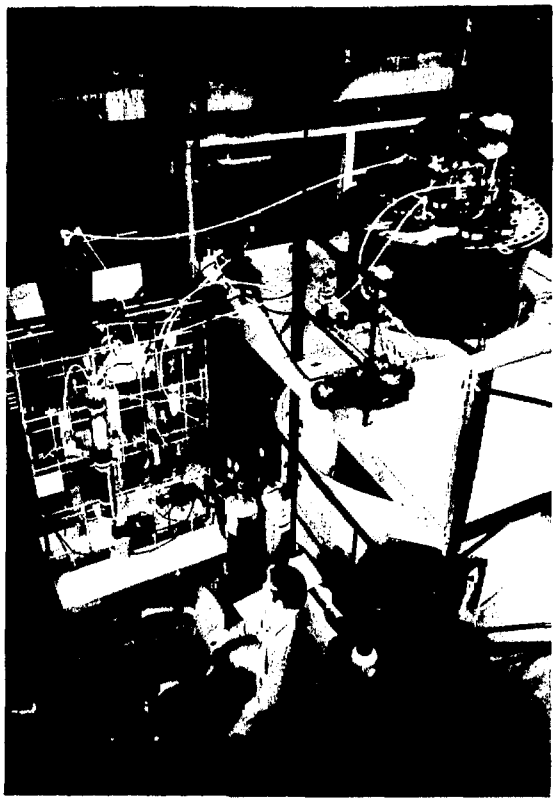


Figure 7. Tank and processing equipment for the 1.3 ton gallium pilot experiment.

The next step on the way to a full scale gallium solar neutrino experiment is a combined absorption cross-section/neutrino oscillation experiment. If neutrinos are shown to oscillate over distances of meters, the result is important. If they do not oscillate, the absorption cross-section can be measured, and the full scale gallium experiment can be performed to determine whether neutrinos oscillate over the sun-to-earth distance or whether the low result of the chlorine experiment has another cause.

RADIOPHARMACEUTICAL RESEARCH

The program in Radiopharmaceuticals is focused on the development of cyclotron-produced positron emitting radionuclides of short half-life (1-110 min) such as carbon-11, oxygen-15,

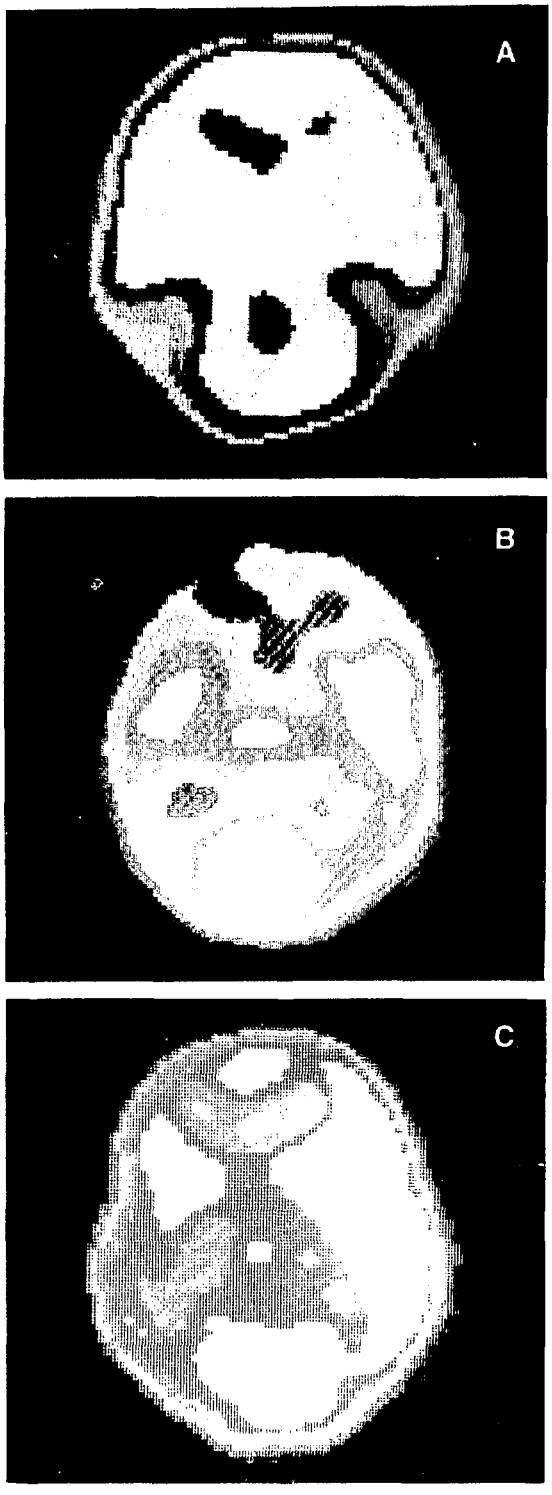


Figure 8. Positron emission transaxial tomographs for (a) normal, (b) schizophrenic, and (c) manic depressive subjects.

nitrogen-13, and fluorine-18, which can be incorporated into materials of medical, biological, or biochemical interest.[22] These new radiopharmaceuticals which are known to have organ or tissue specificity are used in conjunction with a computerized 3-dimensional scanner, the Positron Emission Transaxial Tomograph (PETT), to probe physiological processes and metabolic functions in man.

The radiopharmaceutical, ^{18}F-2-fluoro-2-deoxy-D-glucose (^{18}F-DG), developed at BNL in 1976 is being used in a number of studies in collaboration with investigators from NYU Medical Center on schizophrenia, manic depression, and aging and senile dementia, etc.[23] ^{18}F-FDG mimics the transport of glucose to the brain and permits one to measure the rate of glucose utilization in specific regions of the brain. A data base is being developed for these various disorders.

The illustration (Fig. 8) compares three scans, a normal subject, a schizophrenic, and a manic depressive. Measurements of the glucose metabolic rates in these subjects indicate a trend toward lower than normal glucose metabolism in schizophrenics and a higher than normal rate for manic depressives in the manic phase.

The ^{18}F-FDG methodology holds promise as a quantitative tool which can lead to a facile, rapid and more accurate diagnosis of mental disorders and can aid the physician in prescribing a suitable treatment regimen.

References

1. A. KVICK, R. K. MCMULLAN, and M. D. NEWTON, to be published.
2. T. K. SHAM, J. B. HASTINGS, and M. L. PERLMAN, *J. Amer. Chem. Soc.* **102,** 5904 (1980).
3. M. D. NEWTON in "Structure and Bonding in Crystals", M. O'Keefe and A. Navrotsky, Eds., Academic Press Inc. (1980).
4. D. M. BRENNER, *J. Chem. Phys.* **74,** 494 (1981).
5. A. B. HORWITZ, J. M. PRESES, R. E. WESTON, JR., and G. W. FLYNN, "I.R. multiphoton photochemistry of CF_3Cl", *J. Chem. Phys.* in press.
6. M. A. ANDREWS and K. P. KELLY, submitted to *J. Amer. Chem. Soc.*
7. G. M. BROWN, S.-F. CHAN, C. CREUTZ, H. A. SCHWARZ, and N. SUTIN, *J. Amer. Chem. Soc.* **101,** 7638 (1979).
8. S.-F. CHAN, M. CHOU, C. CREUTZ, T. MATSUBARA and N. SUTIN, *J. Amer. Chem. Soc.*, **103,** 369 (1981).

9. D. C. DEVAULT and B. CHANCE, *Biophys. J.* **6,** 825 (1966).

10. B. CHANCE and M. NISHIMURA, *Proc. Natl. Acad. Sci. USA* **46,** 19 (1960).

11. J. M. OLSON and B. CHANCE, *Biochem. Biophys.* **88,** 26 (1969).

12. D. DE VAULT, J. H. PARKES and B. CHANCE, *Nature* (London) **215,** 642 (1967).

13. P. L. DUTTON, R. C. PRINCE, D. M. TIEDE, K. M. PETTY, K. J. KAUFMANN, T. L. NETZEL, and P. M. RENTZEPIS, *Brookhaven Symposium in Biology No. 28* (ed. J. M. Olson and G. Hind), p. 213 (1976).

14. J. JORTNER, *J. Chem. Phys.* **64,** 4860 (1976).

15. J. J. HOPFIELD, *Proc. Natl. Acad. Sci. USA* **71,** 3640 (1974).

16. D. M. TIEDE, J. J. LEIGH, and P. L. DUTTON, *Biochim. Biophys. Acta* **503,** 524 (1978).

17. I. FUJITA, T. L. NETZEL, C. K. CHANG, and C.-B. WANG (manuscript submitted).

18. C. K. CHANG, *J. Heterocyclic Chem.* **14,** 1285 (1977).

19. J. B. CUMMING, Effects of collectivity on target fragmentation reactions, *Phys. Rev. Lett.* **44,** 17 (1980).

20. R. DAVIS, JR., "Sun" in McGraw-Hill *Yearbook of Science and Technology.*

21. R. DAVIS, JR., B. T. CLEVELAND, and J. K. ROWLEY, Solar neutrino experiments and neutrino oscillations, *VPI Workshop on Weak Interactions as Probes of Unification,* Blacksburg, VA, Dec. 4-6, 1980. To be published in the Am. Inst. of Phys. Conf. Proc. Ser.

22. A. P. WOLF, "Special Characteristics and Potential for Radiopharmaceuticals for Positron Emission Tomography." *Seminars in Nuclear Medicine* **11,** 2-12 (1981).

23. T. FARKAS, M. REIVICH, A. ALAVI, J. H. GREENBERG, J. S. FOWLER, R. R. MACGREGOR, D. R. CHRISTMAN, A. P. WOLF, "The Application of [^{18}F]2-deoxy-2-fluoro-D-glucose and Positron Emission Tomography in the Study of Psychiatric Conditions" in *Cerebral Metabolism and Neural Function,* Chapter 44, J. V. Passonneau, R. A. Hawkins, W. D. Lust, F. A. Welch, Eds. (Williams and Wilkins, Baltimore, MD, 1980), pp. 403–408.

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Medical Department

Biology Department

INTRODUCTION

The Biology Department is involved in fundamental research in molecular genetics, bioenergetics, protein chemistry, and plant science. One goal of this work is to provide information that can be used to evaluate long-term health hazards of expanded energy production. For example, research on DNA replication and repair will allow an assessment of the deleterious effects of ultraviolet light and ionizing radiation, and research on cellular proteases will provide an understanding of the mechanism of pollution-linked respiratory disorders such as emphysema.

Brookhaven provides a unique opportunity for research into molecular details of biological processes. In addition to the scanning transmission electron microscope and the high-field nuclear magnetic resonance spectrometer available in the department, the High Flux Beam Reactor provides facilities for neutron diffraction. The National Synchrotron Light Source (NSLS), expected to start operation in 1981, will provide major facilities for x-ray diffraction and ultraviolet spectroscopy of biological systems. All of these facilities are available for use by visiting scientists from throughout the United States, and have made Brookhaven an important national center for structural research in molecular biology.

MOLECULAR GENETICS

Haemophilus influenzae is a bacterium responsible for most of the acquired mental retardation in the United States. Treatment of infections has been severely compromised recently because of the spread of antibiotic resistance, which usually takes place by transmission of plasmids from cell to cell. When the cells are in a particular physiological state, called competence, plasmids undergo extensive recombination to form multimers such as the one shown in Fig. 1. Electron microscopic investigation of intermediates in such recombination indicates that recombination begins with the asymmetric transfer of a single strand from one molecule to its recombining partner.

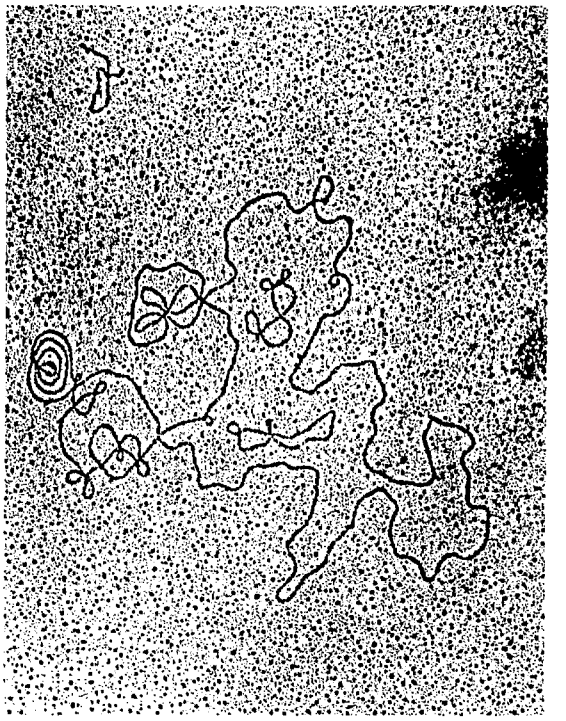

Figure 1. An electron micrograph of plasmids, autonomously replicating small circles of DNA, from *Haemophilus influenzae*. The two smaller structures in the center are monomers and the convoluted multimeric structure is composed of monomers that have undergone recombination. (Magnification is 14,600 ×).

In the presence of visible light, photoreactivating enzymes split cyclobutyl pyrimidine dimers induced in DNA by ultraviolet light. These enzymes are important in the repair mechanism of DNA in human skin. A major obstacle in studying the human enzyme, the low concentration in most easily obtainable human tissue, has recently been overcome by the finding that human lymphocytes stimulated with the mitogen phytohemagglutinin contain high enzyme levels. The stimulated cells serve

as an excellent source for isolation of large quantities of the human enzyme.

Animal cells contain enzymes, called nucleases, that can destroy DNA, but are inhibited from attacking the cell's own DNA. A novel method for detecting and characterizing nucleases after electrophoresis in polyacrylamide gels containing detergent has been applied to the study of these enzymes. A survey of nucleases in the tissues of the rat revealed an enzyme similar to bovine pancreatic deoxyribonuclease I to be present in a number of tissues, most conspicuously in the parotid gland, but also in lymph nodes and urogenital tissues. While the ubiqitous contractile protein actin is a potent inhibitor of the bovine pancreatic and parotid enzymes, actin does not inhibit the analogous rat enzymes. Thus, the actin inhibition of deoxyribonuclease I is species specific and perhaps an accidental occurence without particular biological significance.

BIOLOGICAL STRUCTURE DETERMINATION

Scanning Transmission Electron Microscopy

The Scanning Transmission Electron Microscope (STEM) at Brookhaven is the only instrument of its type able to image single heavy atoms in frozen biological specimens. In the last year research has been directed towards the development of techniques for heavy atom labelling of specific sites in biological molecules. New compounds having clusters of gold or tungsten appear promising, and within the next year it should be possible to locate specific labelled sites in biological molecules with a resolution of about 10 Å.

The STEM is also able to accurately measure mass distribution in complex macromolecular aggregates. This technique has recently been used to establish the structure of fibrinogen, the protein responsible for blood clotting, and to study the molecular details of transcription — the process by which the genetic information stored in DNA is transferred to messenger RNA. In order for transcription to take place a number of protein molecules must bind to a specific region on the DNA molecule, called the "promoter" site. From an analysis of electron micrographs taken in the STEM (see Fig. 2) the total molecular weight of this protein complex can be determined. By combining this measurement with the molecular weight of potential subunits (determined by other methods) the protein subunits required for transcription can be deduced.

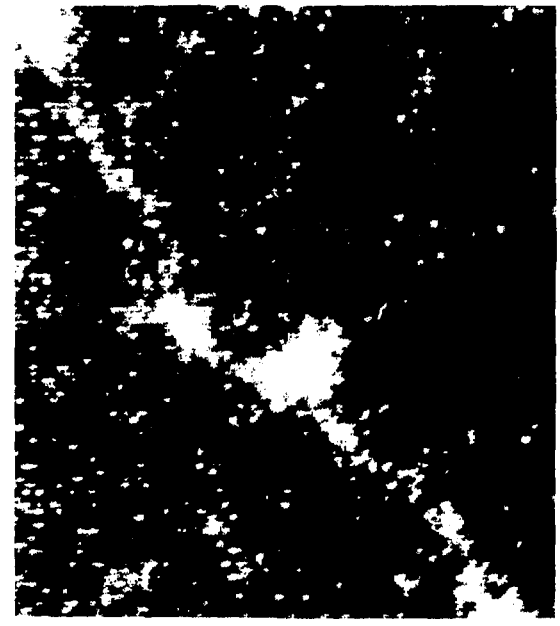

Figure 2. A Scanning Transmission Electron Micrograph of a piece of adenovirus DNA with protein structures bound to it. The largest structure, which is approximately 100 Å by 180 Å, is human RNA polymerase, which copies the genetic information of DNA into messenger RNA. Some of the smaller structures are nucleosomes, which are complexes of histones. Nucleosomes are the basic packaging machinery for DNA in higher animals and may also serve to regulate RNA polymerase function.

Collaborations are also underway with scientists from BNL and other laboratories in studies of filamentous viruses, nucleic acids, membranes, and other biological systems.

National Synchrotron Light Source

The prototype of the Biology Department's Synchrotron Ultraviolet Project spectrometer is already operating at the National Bureau of Standards synchrotron storage ring in Gaithersburg, Maryland. The spectrometer has been used to measure the circular dichroism spectrum of a newly discovered form of DNA (Z-DNA) in the vacuum ultraviolet — a spectral

region inaccessible to conventional spectrometers. X-ray diffraction studies have shown that Z-DNA exists in various forms in the solid state. Circular dichroism spectra are sensitive to the conformation of Z-DNA and will be important in determining which of these various forms exist in solution. The experiment will be moved to the ultraviolet storage ring at the NSLS in 1981.

In collaboration with NSLS and Instrumentation Division personnel the Biology Department is also designing and building a low-angle scattering station which will operate on one of the beam lines of the NSLS x-ray ring. Low-angle scattering probes organization over tens to thousands of angstroms, which is the scale encountered in biological complexes such as ribosomes, muscle fibers, and membranes. While the long exposure times necessary with conventional x-ray sources make it difficult to obtain diffraction patterns from these unstable samples, the high intensity radiation from the synchrotron will allow the rapid acquisition of data and make dynamic studies of biological processes, such as muscular contraction, possible.

Neutron Diffraction

The neutron diffraction facility operated by the Biology Department at the High Flux Beam Reactor, which includes a low-angle spectrometer for scattering experiments and a diffractometer for protein crystallography, is the only installation in this country dedicated to neutron diffraction studies on biological structures. During the last year low-angle scattering experiments have focused on the structure of histone complexes isolated from chromatin, the arrangement of individual proteins within the 30S ribosomal subunit of *E. coli*, and the relative locations of DNA and protein in the filamentous fd DNA-gene 5 protein complex. Protein crystallographic studies have been carried out on trypsin and several derivatives of myoglobin. The neutron analysis of trypsin has led to the resolution of long-standing controversy concerning the structure of serine protease enzymes — identification of the group in the catalytic site (His-57 or Asp-102) that is protonated in the transition state. Figure 3 shows a neutron difference map of the catalytic site of trypsin which clearly shows that the protonated group is His-57.

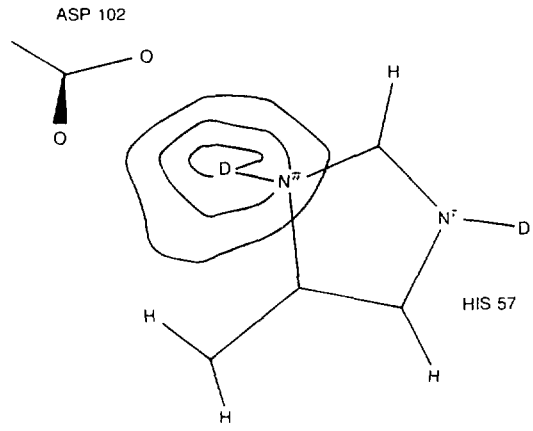

Figure 3. A Neutron Difference map (contoured lines) of the catalytic site of trypsin. The straight-line structures indicate the position of the Asp-102 and His-57 side chains and the contoured lines indicate the position of the deuterium between these two groups. The difference map (contoured lines) clearly indicates that the deuterium is bound to the imidazole ring of His-57.

Nuclear Magnetic Resonance

The high-field nuclear magnetic resonance (NMR) facility in the Biology Department is used for ^{1}H, ^{13}C, and ^{31}P NMR studies of biological systems. In the last year NMR studies in the department have focused on the interaction of divalent cations with membranes. While many important physiological functions are triggered by the calcium-induced fusion of small vesicles with the cell membrane, the molecular details of complexes formed between divalent cations and phospholipids are poorly understood. By using the effects of divalent cations on the NMR spectra of phospholipid membranes some of these details have recently been elucidated. For example, groups in the phospholipid molecules that form ligands for divalent cations have been determined and the contribution of weak "ion-pairs," in which the divalent cations retain their complete hydration shell, has been assessed.

Protein Chemistry

Although proteases, enzymes which specifically cleave portions of protein molecules, are vital to many cellular functions they can be damaging to the cell. For example, in emphysema macrophages or leukocytes liberate proteases that digest the connective tissue of the

lung. Studies in the Biology Department are directed at identifying these proteases and devising ways to inhibit their deleterious effects. A new method has been developed for studying thiol proteases which depends on the ability of specific reagents to combine with the essential sulphydryl group. These techniques have been used to purify a major cellular thiol protease, cathepsin B, and to selectively inactivate thiol proteases in intact macrophages without otherwise damaging the cells.

PLANT SCIENCES

Genetics

The nature of plant gene structure is being investigated in mutants created by movable genetic sequences called "transposable elements". These elements are regulatory portions of chromosomal DNA that can be inserted into any position in the chromosome. A sequence complementary to a portion of the gene for sucrose synthetase in corn has been amplified by cloning in a bacterial plasmid, and has been used as a probe to identify the position of insertion of transposable elements.

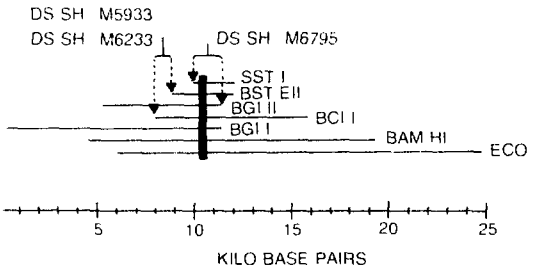

Figure 4. The 25 kilobase region of wild-type chromosomal DNA encoding the sucrose synthetase gene of maize. Each of the horizontal lines above the base line indicates different oligonucleotide fragments produced by digestion of the chromosome with specific restriction enzymes. The heavy vertical bar indicates the site of hybridization to the cloned sequence of DNA and the dashed lines indicate the position of transposable elements in several mutants.

Nucleases called "restriction" enzymes are used to cleave the chromosomal DNA into fragments and to determine the position of the transposable elements in the fragments (see Fig. 4). These fragments can then be positioned relative to each other by alignment of the section that hybridizes to the radioactively labelled cloned sequence (thick vertical bar), and the position of the transposable elements in the gene can thus be determined.

Regulation of Cell Cycle Division

When a plant cell divides, each daughter cell inherits an identical set of genes that are located in the DNA of the chromosomes. In pea, each of the diploid cells has 14 chromosomes and each chromosome has two DNA molecules about 17 cm long. Work in the Biology Department has shown that, several hours before cell division, the long molecules are replicated in an organized, step-wise fashion by units called replicons. At the onset of replication, groups or clusters of about 18 replicons, aligned in tandem on the same molecule, begin producing a new DNA chain. Each replicon of a cluster starts nearly simultaneously, as if responding to a particular signal. Meanwhile, other clusters, flanking the active one, remain quiescent until they too are signaled to start. The cascading, ordered activity of the clusters continues until a new replica of the 17 cm molecule is nearly complete. Then, the unattached DNA chains between neighboring clusters and replicons are joined end-to-end producing a contiguous DNA molecule ready to be folded into a chromosome and eventually distributed to a daughter cell.

Electron Microscopy

Although cellulose, with its high energy content, is the most abundantly produced substance of the biosphere, the details of how it is formed at the protoplasmic surface of plant cells are just beginning to be understood. It is believed that microtubules, slender proteinaceous elements of the cytoplasm some 24 nm in diameter, are involved in determining the direction in which microfibrils of cellulose are synthesized at the plasma membrane of the cell. The distribution of connections between the microtubules and the plasma membrane has been determined recently for flax fibers using serial thin sections studied by electron microscopy. The connections, probably single protein molecules, are more frequent than previously recognized and are probably involved in the way the synthesizing apparatus moves in the plasma membrane during deposition of the cellulose.

* * *

Only a fraction of the groups in the department have been represented in this brief summary. For more information, the following departmental roster and bibliography selected from the more than ninety articles published between October 1979 and September 1980 can be consulted.

Selected Publications

F. E. AHMED, A. GENTIL, B. S. ROSENSTEIN, and R. B. SETLOW, DNA excision repair in human cells treated with ultraviolet radiation and 7, 12-dimethylbenz(a)anthracene 5, 6-oxide. *Biochim. Biophys. Acta* **608,** 154-166 (1980).

C. W. ANDERSON, and J. B. LEWIS, Amino-terminal sequence of adenovirus type 2 proteins: hexon, fiber, component IX, early protein 1B-15K. *Virology* **104,** 21-41 (1980).

F. A. BURR, and B. BURR, "The cloning of zein sequences and an approach to zein genetics," in *Genome Organization and Expression in Plants,* C. J. Leaver, Ed. pp. 227-231, Plenum 1980.

S. M. D'AMBROSIO, and R. B. SETLOW, Modulation by caffeine of enhanced postreplication repair in mammalian cells treated with N-acetoxy-acetylaminofluorene. *J. Environ. Path. Toxicol.* **4,** 181-191 (1980).

J. J. DUNN, and F. W. STUDIER, The transcription termination site at the end of the early region of bacteriophage T7 DNA. *Nucleic Acids Res.* **8,** 2119-2132 (1980).

W. KIM, and C. LEDBETTER, Surface morphology of *Trichinella spiralis* by scanning electron microscopy. *J. Parasitol.* **66,** 75-81 (1980).

G. KING, W. STOECHENIUS, H. CRESPI, and B. SCHOENBORN, The location of retinal in the purple membrane profile by neutron diffraction. *J. Mol. Biol.* **130,** 395-404 (1979).

A. A. KOSSIAKOFF, and S. A. SPENCER, Neutron diffraction identifies his-57 as the catalytic base in trypsin. *Nature* (London) **288,** 414-416 (1980).

H. Z. HILL, and R. B. SETLOW, Postreplication repair in three murine melanomas, a mammary carcinoma, and a normal mouse lung fibroblast line. *Cancer Res.* **40,** 1867-1872 (1980).

A. LAU, A. C. MCLAUGHLIN, R. C. MACDONALD, and S. G. A. MCLAUGHLIN, "The adsorption of alkaline earth cations to phosphatidyl choline bilayer membranes: a unique effect of calcium," in *Bioelectrochemistry: Ions, Surfaces, Membranes,* M. Blank, Ed., pp. 49-56, *Advances in Chemistry Series,* **188,** American Chemical Society, Washington, D.C. (1980).

A. C. MCLAUGHLIN, H. TAKEDA, and B. CHANCE, Rapid ATP assays in perfused mouse liver by ^{31}P NMR. *Proc. Nat. Acad. Sci.* (USA) **76,** 5445-5449 (1979).

P. B. MOORE, "Scattering studies of the three-dimensional organization of the *E. coli* ribosome," in *Ribosomes. Structure and Genetics,* G. Schambliss, G. R. Craven, J. Davies, R. Davis, L. Kahan and M. Nomure, Eds., pp. 111-113, University Park Press, Baltimore, 1980.

N. K. NOTANI, and J. K. SETLOW, An inducible repair system in *Haemophilus influenzae* unaccompanied by mutation. *J. Bacteriol.* **143,** 516-519 (1980).

M. RIGBI, J. ROSINSKI, H. W. SIEGELMAN, and J. C. SUTHERLAND, Cyanobacterial phycobilisomes: selective dissociation monitored by fluorescence and circular dichroism. *Proc. Natl. Acad. Sci.* **77,** 1961-1965 (1980).

A. L. ROSENTHAL, and S. A. LACKS, Complex structure of the membrane nuclease of *Streptococcus pneumoniae* revealed by two-dimensional electrophoresis. *J. Mol. Biol.* **141,** 133-146 (1980).

R. B. SETLOW, "DNA repair pathways." in *DNA Repair and Mutagenesis in Eukaryotes,* W. M. Generoso, M. D. Shelby, and F. J. deSerres, Eds., pp. 45-54, Plenum, New York, (1980).

R. B. SETLOW, Damages to DNA that result in neoplastic transformation. *Adv. Biol. Med. Phys.* **17,** 99-108 (1980).

R. B. SETLOW, and F. E. AHMED, "DNA repair in human cells exposed to combinations of carcinogenic agents." *Carcinogenesis: Fundamental Mechanisms and Environmental Effects,* B. Pullman, P. O. P. Ts'o, and H. Gelboin, Eds., pp. 453-464, D. Reidel Pub. Co., Boston, 1980.

E. SHAW, and R. T. DEAN, The inhibition of macrophage protein turnover by a selective inhibitor of thiol proteinases. *Biochem. J.* **186,** 385-390 (1980).

R. E. SLOVACEK, and G. HIND, Energetic factors affecting CO_2 fixation in isolated chloroplasts. *Plant Physiol.* **65,** 526-532 (1980).

F. W. STUDIER, A. H. ROSENBERG, M. N. SIMON, and J. J. DUNN, Genetic and physical mapping in the early region of bacteriophage T7 DNA. *J. Mol. Biol.* **135,** 917-948 (1979).

B. M. SUTHERLAND, L. C. HARBER, and I. E. KOCHEVAR, Pyrimidine dimer formation and repair in human skin. *Cancer Res.* **40,** 3181-3185 (1980).

B. M. SUTHERLAND, and S. G. HAUSRATH, Insertion of *E. coli* photoreactivating enzyme into mammalian cells. *Nature* **286,** 510-511 (1980).

J. C. SUTHERLAND, B. M. SUTHERLAND, G. D. CIMINO, and K. P. GRIFFIN, Photoreactivating enzyme from *E. coli*: Interactions with DNA and mechanism of action. *Biophys. J.* **32,** 242-243 (1980).

J. C. SUTHERLAND, and B. HOLMQUIST, Magnetic circular dichroism of biological molecules. *Ann. Rev. Biophys. Bioeng.* **9,** 293-326 (1980).

J. VANT HOF, Pea (*Pisum sativum*) cells arrested in G2 have nascent DNA with breaks between replicons and replication clusters. *Exptl. Cell Res.* **129,** pp. 231-237 (1980).

G. J. WAGNER, "The subcellular site and nature of intracellular Cd in plants." in *Trace Substances in Environmental Health*, D. D. Hemphill, Ed., Vol. XIII, p. 115-123, University of Missouri Press, (1979).

J. S. WALL, and J. F. HAINFELD, Mass measurement with the STEM-Biological applications. *Proc. 38th EMSA Meeting, San Francisco,* G. W. Bailey, Ed., pp. 674-675, Claitors Publishing Div., Baton Rouge LA, (1980).

W. B. WITTEN, J. M. OLSON, and R. M. PEARLSTEIN, Seven-fold exciton splitting of the 810-nm band in bacteriochlorophyll *a*-proteins from green photosynthetic bacteria, *Biochim. Biophys. Acta,* **591,** 203-207 (1980).

A. D. WOODHEAD, and R. B. SETLOW, "Response to and recovery from acute sublethal gamma radiation in the Amazon molly, *Poecilia formosa.*" in *Radiation Effects on Aquatic Organisms*, N. Egani, Ed., pp. 171-182, Jap. Sci. Soc. Press, Tokyo, (1980).

M. YEAGER, B. P. SCHOENBORN, D. E. ENGELMAN, P. MOORE, and L. STRYER, Neutron diffraction of intact retinas. *J. Mol. Biol.* **137,** 315-348 (1980).

BIOLOGY DEPARTMENT

Richard B. Setlow, Chairman
Geoffrey Hind, Deputy Chairman

Molecular Genetics

Carl W. Anderson
Organization and expression of the adenovirus genome.

John J. Dunn
Synthesis and processing of RNA in E. coli and its phages; role of RNase *III* in RNA processing.

Sanford A. Lacks
Mechanism of genetic transformation in *S. pneumoniae;* function of DNases.

Jane K. Setlow
Transformation, recombination and repair in *H. influenzae* and its phages.

Richard B. Setlow
Damage to DNA by radiation and chemical carcinogens and its repair.

F. William Studier
Genetics and physiology and bacteriophage T7; gene expression, DNA metabolism, phage assembly.

Betsy M. Sutherland
DNA repair; cellular level photobiology.

Biological Structure Determination

R. Douglas Carlson
Neutron scattering studies of chromatin and histone complexes.

Marshall Elzinga
Muscle and microtubular protein chemistry.

Paul V. C. Hough
Transcription in eukaryotes.

Anthony A. Kossiakoff
Protein crystallography by neutron and x-ray diffraction.

Alan C. McLaughlin
High resolution NMR studies of membrane structure.

Benno P. Schoenborn
Neutron diffraction of biological structures; ribosomes, membranes.

Elliott N. Shaw
Structure and function of cellular and blood proteases; enzyme chemistry.

John C. Sutherland
Optical probes of macromolecular conformations and interactions.

Joseph S. Wall
High resolution scanning transmission electron microscopy and single atom staining of filamentous viruses.

David S. Wise
Small angle x-ray and neutron scattering studies of biological receptor structure.

Bioenergetics

Geoffrey Hind
Photosynthetic electron transport and phosphorylation; ion fluxes in chloroplasts and plant cell vacuoles.

John M. Olson
Structure of the photosynthetic unit of green bacteria.

Plant Sciences

Benjamin Burr; Frances A. Burr
Biochemical genetics and storage protein synthesis in maize.

Myron C. Ledbetter
Electron microscopy of DNA, other biomolecules, and fine structure of plant cells.

Lloyd A. Schairer
Plant mutagenesis.

Daniela Sciaky
Genetic engineering in plants.

H. William Siegelman
Phytoplankton physiology and biochemistry.

Harold H. Smith
Use of cell and tissue culture in plant cell genetics.

Jack Van't Hof
Genetics and regulations of the plant cell division cycle.

George J. Wagner
Characterization of plant cell vacuoles; mechanisms of accumulation in plant cells.

At the close of Fiscal 1980 eighteen postdoctoral Research Associates, some supported by outside grants or fellowships, were contributing to the research efforts of many of the groups listed above.

Medical Department

INTRODUCTION

The Medical Research Center (Medical Department) contains three major divisions: the Hospital, the Research Laboratories, and the Occupational Medicine Clinic which serves Brookhaven National Laboratory. Basic science in biology, chemistry, and physics is directed toward application of research findings to clinical medicine. The Hospital of the Medical Research Center, a hospital devoted entirely to research patients, supports clinical studies in areas which include: respiratory diseases; neuropsychiatric disorders; hematological disease (e.g., chronic lymphocytic leukemia); cardiopulmonary disorders; hepatobiliary dysfunction; cancer of many types, including malignant ocular melanoma; toxicological problems of many kinds; bone and mineral metabolism; and dietary and nutritional disorders. Research efforts are also made to improve therapeutic measures for disease: brain tumor therapy through boron capture of epithermal neutrons, and proton beam irradiation; extracorporeal irradiation of blood in leukemia; iron chelator efficacy in thalassemia; and nonsurgical treatment of ocular melanoma. Earlier diagnoses, and studies of the mechanism of disease are approached through medical applications of nuclear technology (which includes nuclear medicine techniques such as positron emission tomography).

The ability of the Department to attempt and accomplish these various scientific goals which are directly, or will ultimately be, concerned with human disease is due to (1) the excellent cadre of skilled scientists in the Department and the Laboratory; (2) the freedom and ease with which one may collaborate and consult with scientists in other departments; (3) the maintenance of laboratory service divisions of high quality which enable prototype fabrication, design, and instrument maintenance and repair to be obtained quickly; and (4) the unique facilities and instrumentation existing in the Medical Department and the Laboratory—facilities which are costly, or large, or unique by way of design and capability.

The Research Hospital of the Medical Research Center, although reduced in capacity from 44 beds (in the mid-'60s) to 11 beds today, is still equipped and staffed to carry out the research projects outlined above. This facility, though not unique in itself, must be considered as most unusual—by virtue of its association with a research laboratory and major facilities and devices, such as particle accelerators, reactors, and highly-unusual or unique and complex diagnostic tools.

The Medical Department as part of Brookhaven National Laboratory is a national resource for research and training and may be called upon by the Department of Energy (DOE) to solve specific problems affecting the national health and welfare. Maintenance of the excellence of this institution is thus most important to its readiness and capability to respond to such requests. Exemplary of this capability has been the Department's responsiveness to recent mission changes as the Department of Energy evolved from ERDA and the AEC. Core scientific capability has been maintained—but at a lower level due to DOE budget limitations.

Relatively new efforts in the Department center on toxicology, respiratory physiology, and pathology related to pollutants derived from energy production; cytogenetic studies and genetic studies at the request of DOE and EPA; clinical and animal studies of health effects related to fossil fuel technologies at the request of DOE, EPA, and NIH; and new screening mechanisms for determination of health effects of pollutants and health effects related to photovoltaic technologies.

The following report, although brief, gives some idea of the types of work being done. Additional information may be obtained from publications of the Department.

HEALTH ASPECTS OF PHOTOVOLTAIC TECHNOLOGY

The growing use of photovoltaic cells in energy production poses new questions regarding possible health effects of this technology to the general public. The photovoltaic (PV) devices that convert sunlight directly into electricity are semiconductors which produce a voltage and, if connected to a load, an electric current, when sunlight falls on them. Most PV cells contain at least one chemical element which either is known to be toxic (e.g., arsenic or cadmium) or about which only little health-effects information exists (e.g., indium or gallium). These elements vary in concentration from a few parts per million to major fractions of the matrix.

The Department of Energy is anxious to ensure that potential hazards are identified at a stage sufficiently early to permit their elimination either through devising a satisfactory solution or through redirecting the technology development. To accomplish this, it has established a "Field Center" at Brookhaven to identify potential problems involving not only human health but also the environment, safety, and the technology used in controlling environmental releases. The Center will seek to mitigate these problems by various means such as in-house or subcontracted research, and recommendations to technology developers. Brookhaven's Department of Energy and Environment (DEE) is providing the management of the overall program as well as the detailed programmatic effort for the environmental, safety, and control technology areas, and the Medical Department provides assistance in the areas of health problems and health-effects research.

Specific objectives of the medical effort include identification of existing or potential problems, identification of missing information needed to quantify such problems and specific areas in which PV health-effects is needed, definition of a program to accomplish this additional research and recommendation of appropriate priorities, and providing advice on a variety of matters such as interpretation of results and resolution of conflicting data, etc.

The Proceedings of a workshop on Health Effects of Photovoltaic Energy, which brought to Brookhaven many experts representing a broad spectrum of disciplines, was published in June, 1980. This definitive volume provided the basis for discussions which led to a health-effects research plan, which was recommended to DOE for 1981 and subsequently expanded into a five-year plan. While awaiting implementation of this plan, the program continues to monitor the development of PV technology and the status of health-effects/toxicity information for the purpose of identifying new potential problems and updating the estimated seriousness of those already identified.

INTERACTIONS OF DIETHYLSTILBESTROL AND X-IRRADIATION ON MAMMARY TUMOR INDUCTION IN RATS

The intent of this study was to investigate the relationship between the dose of diethylstilbestrol (DES) and its synergistic interaction with x-irradiation for mammary carcinogenesis in ACI rats. In addition, the role of pituitary prolactin secretion in this synergism was studied. Ten groups of approximately 25 female ACI rats, 84-91 days of age, were implanted with a compressed 20 mg pellet containing either 5, 1.67, 0.56, 0.19, or 0 mg of DES combined with cholesterol. Two days later, one group at each DES dose level was exposed to 150 R of 250 kVp total-body x-radiation. Plasma prolactin levels were determined by radioimmunoassays taken at approximately 100-day intervals. The experiment was terminated at 659 days after pellet implantation. Two basic types of mammary gland carcinogenic response were found: either individual mammary adenocarcinomas, or multiple adenocarcinomas consisting of 4 or more carcinomas within a single quadrant of mammary gland tissue. Increasing the dose of DES (with or without irradiation) increased the incidence of rats with an adenocarcinoma as well as the number per rat, while at the same time decreasing the mean time to appearance. Multiple carcinomas were found only in rats with the two highest doses of DES (with or without irradiation) and this response appeared to be DES dose-dependent. Combining radiation with DES treatment (except at the lowest DES dose) produced a synergistic increase in the incidence of rats with individual and multiple mammary adenocarcinomas, and number per rat, and de-

creased the time to appearance. Rats receiving x-rays alone had only a few late-appearing mammary adenocarcinomas while none were seen in the cholesterol control group. Almost all the rats in the three highest-dose groups had pituitary tumors, while in all other groups only about one-half of the animals had these tumors. There appeared to be a definite relationship between the dose of DES and both the initiation and the degree of plasma prolactin elevation for all DES doses except the lowest. These data suggest that in female ACI rats, mammary adenocarcinoma induction by DES alone or by the synergistic interaction of DES and x-irradiation is highly DES dose-dependent. This DES dose dependence appears to be mediated via an estrogenic stimulation of prolactin secretion, since the higher and the earlier that prolactin was elevated the greater were the individual and multiple mammary adenocarcinoma responses.

REGULATORY MECHANISMS OF ERYTHROPOIETIN PRODUCTION

The regulation of red cell production in man is of major concern because of the wide variety of disease states which occur in man, either because of a deficiency or excess of red blood cells. These conditions are commonly referred to as anemia or polycythemia. Prior to the advent of a radioimmunoassay (RIA) for erythropoietin (Ep) one could only speculate about the levels of the hormone Ep in many clinical disease states associated with the abnormal production of red blood cells. Ep is considered by many to be the primary regulator of red cell production and its production is stimulated by tissue hypoxia. Others have postulated that there may be other regulators and/or inhibitors of red cell production. It has been our intent over the past year to define the levels of this hormone in normal man as well as in subjects with chronic pulmonary disease.

In a collaborative study with Dr. Joseph F. Garcia of the Lawrence Berkeley Laboratory, Ep levels were measured in 309 BNL employees. The mean ± 1 SD level of immunoreactive Ep in males was 17.0 ± 5.7 mU/ml and in females was 18.7 ± 7.0 mU/ml. Serum levels of the hormone were also measured in an additional 48 normal volunteers in order to determine if there were age-related differences in levels of the hormone. The results of this study indicated to us that there was no obvious effect of age on the level of the hormone. Studies directed toward measuring diurnal variations as well as the effect of exercise on the level of the hormone were also conducted, and clearly demonstrated that normal men and women do not exhibit diurnal variations in the hormone level nor does exercise influence the level of the hormone.

Residents of high altitudes and patients with cyanotic congenital heart disease, with right to left shunting of blood, typically develop secondary polycythemia generally commensurate with the degree of hypoxia to which they are subjected. However, patients with chronic lung disease have eluded simple categorization. While some patients with hypoxemia secondary to chronic lung disease develop secondary polycythemia, others do not. Patients with chronic lung disease were studied in order to determine if their serum levels of immunoreactive Ep correlated with the pO_2, O_2 saturation, O_2 content, pH, carboxyhemoglobin level, or red cell mass. Their levels of immunoreactive Ep were compared to levels obtained in an age-matched group of "normals". Sequential levels of Ep were also determined over a 48-hour time interval in 30 subjects with chronic lung disease.

Most subjects with chronic lung disease in the present study did not have increased serum levels of immunoreactive Ep compared to the control population. The only significant correlation observed was between the carboxyhemoglobin level and the serum level of immunoreactive Ep. Subjects with chronic lung disease did exhibit diurnal variations in Ep levels with peak levels on 2 consecutive days occurring at midnight.

The diurnal pattern of serum levels of immunoreactive Ep which we observed was contrary to what was anticipated. Since it is known that arterial oxygen saturation levels fall during sleep, in subjects with chronic lung disease diurnal variations in Ep levels were expected to occur in the early morning hours of the day. The pattern observed in subjects who were cigarette smokers was anticipated since the level of carboxyhemoglobin increases as the day progresses. That this is not the sole explanation is evidenced by the fact that several subjects who

were nonsmokers exhibited identical patterns. The population of chronic lung disease subjects in the present study did not have significant arterial oxygen desaturation and they maintained a normal arterial O_2 content. The added insult of an increased carboxyhemoglobin in some subjects may have been sufficient to alter O_2 transport in such a manner that Ep levels were increased. We have demonstrated that fluctuations in Ep levels occur in subjects with hypoxemia, and in this respect they differ from residents of high altitude and patients with congenital cardiac disease in whom the degree of hypoxemia is relatively constant. Sustained elevations of Ep may be required before the red cell mass increases. One question which has never been satifactorily answered relates to how much Ep is required to increase the red cell mass. Alternative explanations for our findings might be that Ep inhibitors are present in subjects with chronic lung disease or that what was measured as immunoreactive Ep in our study was not biologically active Ep.

PULMONARY PROGRAM

The object of both the clinical and experimental areas of research in the pulmonary program is to develop and define more sensitive techniques for assessing respiratory disease, and to assess the health effects of energy-related atmospheric pollutants.

The clinical studies, conducted in healthy individuals and in patients with a variety of pulmonary disorders, are performed in the Medical Research Hospital. Our hospital contains some of the most modern technology available for evaluating human respiratory function, including the use of nuclear medicine techniques to measure radioactive tracers in inspired gases and in pulmonary blood. These techniques can provide highly sensitive and accurate measurements of early injury to small airways and terminal lung units.

The probable transition back to coal as a major source of energy in the next few decades may cause significant health problems. Not only is there the potential of adverse health effects associated with the mining of coal, but also with the atmospheric pollution resulting from processing and burning the coal. Therefore, it is important to design clinical studies which identify and define specific susceptible populations, and also to develop pertinent animal models of human respiratory disease for more intensive mechanistic studies.

One of the major goals of the clinical program has been to measure changes occurring in miners exposed to coal dust, and to correlate these findings with the degree of exposure. A comprehensive study, in collaboration with Marshall University, the Appalachian Pulmonary Laboratory, and the University of California, has started. To date, we have quantified respiratory dysfunction in a group of retired coal miners. Despite normal chest films in some of the patients, our more sensitive techniques have shown pulmonary impairment in the peripheral lung units of all miners, including abnormal ventilation and gas exchange, and obstructed small airway flow. Studies of regional ventilation and perfusion in chronic pulmonary disease, using nuclear medicine techniques, have resulted in the development of a unique dual approach to assess pulmonary status. Through the combination of data from mismatched ventilation and perfusion ratios, and objective numerical indices from image measurements, very early pulmonary dysfunction can be identified. This technique has been applied to the diagnosis of emphysematous patients and retired coal miners and with it we can detect early abnormalities despite a normal chest x-ray. Future work in this area will be directed towards increasing the sensitivity of measurements and developing protocols to correct data for motion and tissue attenuation.

In another clinical program, the deposition, translocation, and clearance of inhaled particles in the human lung has been investigated using a gamma camera and particles tagged with radioisotopes. Results have confirmed the previously reported biphasic alveolar clearance mechanism and have been extended to show that clearing appears to be independent of particle penetration. This suggests the involvement of only a single pulmonary anatomic compartment. Additional studies have indicated that cigarette smoking interferes with both phases of clearance, and upcoming projects will be expanded to study alveolar removal of larger particles.

Epidemiologic studies have shown clearly that people at high risk during episodes of ex-

cessive air pollution are those who are already compromised by lung disease. To better understand the mechanisms whereby these diseased individuals are at greater risk, we are continuing our efforts to develop animal models of respiratory disease. We are currently working with bleomycin and oxygen in order to produce a model of pulmonary fibrosis in rats. Our plan is to then see if exposure to other materials alters the fibrotic response, or if animals with pre-existing fibrosis will develop other pulmonary disease when exposed to air pollutants.

Several projects are underway in which the relationship between hypertension and air pollution is investigated. At Brookhaven, the relationship between environmental factors and hypertension has been under study for several years and this is an outgrowth of those studies. We have shown that exposure to sulfur dioxide (SO_2) does not alter the course of hypertension in susceptible animals. On the other hand, animals susceptible to salt-induced hypertension are also extremely sensitive to ozone exposure. This observation has been repeated with acrolein and it appears that animals susceptible to salt-induced hypertension are also susceptible to a variety of other environmentally-induced stresses.

The recent evidence proving asbestos to be a carcinogen has shifted focus to the use of fiberglass for a variety of insulation purposes. However, recent reports have suggested the fiberglass possibly produces fibrosis in the lung, and also has the potential to produce the same kinds of tumors that asbestos produces; namely, mesotheliomas. The studies suggest that the physical size of the fiber, particularly the length, may play a very important role in the carcinogenic potential of the fiber. We are, therefore, investigating the mammalian pulmonary response to the introduction of specifically sized ($1.5 \times 60\ \mu m$ or $1.5 \times 5\ \mu m$) glass fibers into the respiratory tract of rats. This extensive study evaluating the behavior of sized glass fibers as a function of the fiber size, the dose, and the route of administration has been underway for some time. Our results using a radioactive label show little difference in the rate of removal of long vs. short fibers from the animal. The method is not sufficiently sensitive to see the exact location of the fibers within the lung. The histological response to long vs. short fibers is different. The short fibers are totally phagocytized by alveolar macrophages with some translocation to regional lymph nodes. Long fibers were not completely engulfed by phagocytic cells, were not transported to lymph nodes, and were associated with foreign body granulomas in the lung. Comparison is now being made of the distribution of fibers after intratracheal instillation with the distribution of fibers after inhalation. Exposures have been completed and the results will be forthcoming soon. We have evaluated some of the tissue using a scanning electron microscope. Figure 1 shows a scanning electron micrograph of a rat lung following intratracheal instillation of short glass fibers. It is clear that clusters of fiber-containing macrophages are seen in several alveoli. Figure 2 is a higher power photograph showing that almost all of these short fibers are observed to be inside phagocytic cells which are presumed to be alveolar macrophages. In contrast, Fig. 3 shows that long fibers cannot be engulfed by single macrophages. The macrophages line up along the fibers in an attempt to engulf them, but because of the length are unsuccessful.

The assessment of pulmonary function in small animals is an important objective and one we feel is prerequisite to a meaningful study of toxic lung injury. Our laboratory for measuring pulmonary function in rodents has been operational throughout this year. Significant advances have been made in the computerized

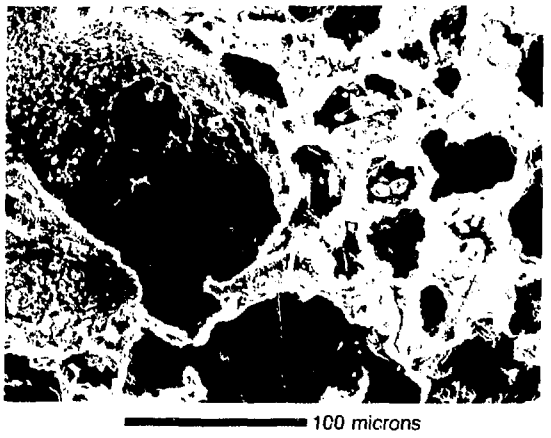

Figure 1. Scanning electron micrograph of rat lung following the intratracheal instillation of glass fibers. Clusters of fiber-containing macrophages occupy the lumina of several alveoli.

Figure 2. Scanning electron micrograph showing macrophages which have completely engulfed the short fibers. A solitary longer glass fiber is only partially phagocytized.

Figure 3. Scanning electron micrograph illustrating the incomplete attack of macrophages on long fibers of glass. The incomplete removal of these fibers may be related to potential tumor development.

collection and management of the data associated with pulmonary function. It is now possible to assess the elastic properties of pulmonary tissue, diffusion capacity, and ventilation distribution aspects of the lung. These values, coupled with the dynamic flow volume measurements and blood gas analyses, can all be repeated serially on the same animal. To date, these results have provided insight into lung injury following exposure to ozone, acrolein, sulfur dioxide, and other energy-related air pollutants.

EFFECTS OF ENVIRONMENTAL POLLUTANTS ON RESPIRATORY FUNCTIONS AND PULMONARY DEFENSE MECHANISMS

The lung is composed of several million small air sacs lined by delicate tissue membrane separating air from blood. This extensive respiratory membrane is exposed directly to a variety of air-borne pollutants. The inhaled pollutants encounter a variety of pulmonary defense mechanisms. The major aim of this research is to better understand the organismal and cellular mechanisms controlling respiratory functions and lung host-defenses, and how these functions are altered by environmental pollutants. A secondary aim is to elucidate the nature of the perturbations in human lung host-defenses responsible for the increased susceptibility to inhaled pollutants.

Infections of the respiratory tract account for a large portion of the total illness in the general population and there is good evidence in both children and adults that the incidence of respiratory disease is proportional to air pollution levels. The effects of inhaled pollutants on pulmonary defense mechanisms are currently being studied using sheep as experimental subjects. Sheep offer several advantages over the frequently used laboratory rodents. For example, some anatomical features of the respiratory tract are remarkably similar to that of man, including the presence of respiratory bronchioles, which are reported to be extremely sensitive to inhaled irritants. In addition, the size of the animal permits serial sampling and analysis of fluid and cellular compartments which are important in host defense of the lung, e.g., lung lavage, pulmonary lymph, blood, bone marrow, and lung tissue. This in turn allows a comprehensive evaluation in individual animals before, during, and following exposure to air-borne pollutants. The technique for serial cell (and fluid) sampling and analysis and the technique for pollutant exposure are well developed and experiments focusing on the effects of inhaled NO_2 on pulmonary defense systems have begun. The initial exposures were at the level of 5 ppm, 1½ h a day, for 2 weeks. This exposure regimen resulted in a decrease in the number of antibody-forming cells in pulmonary lymph following intrabronchial immunization.

The effect was of short duration and may involve injury to a cell type which is rapidly replaced. Most other parameters studied were unaffected by these exposures.

Oxidative pollutants such as NO_2, SO_2, and O_3 produce interstitial and alveolar edema. The precise site and nature of injury resulting in pulmonary edema are unknown. Alveolar edema (flooding of air sacs) does not occur until the late stage of the disease process. This research employs combined use of computer-based simulation (in collaboration with members of the Division of Pulmonary Medicine, SUNY at Stony Brook) and sheep with experimentally induced edema, in order to provide early indicators of developing permeability perturbations in the respiratory air exchange membranes. Hydrostatic and oncotic pressure changes are induced by intravenous infusions of appropriate fluids. Mechanical obstruction to pulmonary blood flow is provided by distending a balloon on a catheter in the left atrium. Membrane permeability is perturbed by a variety of pharmacological agents. The early results obtained from this combined approach are encouraging. Definitive studies are planned to elucidate the mechanisms of pollutant-induced injury at the enthothelial-interstitial and interstitial-epithelial barriers of the respiratory membranes.

Pulmonary emphysema is a frequent late sequela of oxidative pollutant-induced lung injury. The currently available diagnostic modalities do not permit detection of human lung damage prior to irreversible structural changes. It is generally agreed that emphysema is a result of an imbalance in the elastase-antielastase system leading to abnormal catabolism of lung elastin. In this research (in collaboration with Dr. A Janoff, Dept. of Pathology, SUNY at Stony Brook) secretion of desmosine, an elastin-specific peptide, is measured by a highly sensitive radioimmunoassay. Pancreatic elastase is instilled into lungs. Desmosine levels in serum, urine, lung lymph, and lung lavage are measured at various time intervals following enzyme treatment. The preliminary results show that determination of desmosine excretion may permit detection of developing structural lung damage prior to the stage of irreversible injury. This approach is expected not only to be useful in detection of early lung damage in man, but may also make it possible to investigate the mechanisms underlying pollutant-induced lung injury in experimental animals.

NUCLEAR MEDICINE

The Nuclear Medicine Program in the Medical Department attempts to link new scientific and engineering techniques, insights, and developments to the improvement of medical diagnosis and therapy. Important developments at BNL in accelerator design (MEQALAC), instrumentation (multiwire proportional chambers with electronic collimators), and the acquisition of improved data collection and analysis systems for imaging research have established the ground work for important future developments. Specific accomplishments from last year's work that we "highlight" are: (1) Quantitative Autoradiography with Radiopharmaceuticals, and (2) Radiation Therapy of Malignant Melanoma.

(1) Quantitative Autoradiography With Radiopharmaceuticals

The increasing availability of medical cyclotrons and positron emission transaxial tomography (PETT) systems requires the development of new radiopharmaceuticals capable of providing quantitative metabolic information in normal and diseased organs. Analysis of the relative merits of new radiopharmaceuticals is facilitated by the comparison of the biodistribution of multiple tracers imaged simultaneously. Accepted tracers serve as the reference against which the merits of the new agents are assessed. This comparison is being accomplished using a new large-section (whole body or entire organ) autoradiography (ARG) sample preparation system, in conjunction with quantitative videodensitometry.

A typical experiment involves the analysis of the distribution of short-lived tracers (typically β^+-emitters) and longer-lived tracers (typically low energy β^- emitters). A mixture of the two labelled compounds may be administered to an animal simultaneously to validate the biodistribution of a new β^+-labelled compound in comparison to the well characterized ^{14}C-labelled compound. Or, these two compounds can be given in temporal sequences which permit

analysis of the effects of intervening stimuli. β activities of different energies (viz. ^{14}C and ^{3}H) are being estimated by exposing ARG films for different periods and with selection of interposing filters before measuring the densities, or by digital image subtraction. Improved methods of separating the images from these two low energy β emitters are under development.

Quantification of the ARG is usually accomplished by taking point-by-point measurements with a conventional manually operated optical densitometer. We are quantifying the ARG and achieving high spatial resolution, by using a minicomputer-based videodensitometer. Digital images of the ARG, along with several standard samples of known amounts of radioactivity, are obtained using a video camera equipped with a zoom lens to make the measurements which are stored digitally. Such digitized sampling provides 256x256, 512x512, or even 1024x1024 picture elements in each field. Accordingly, a 1 cm^2 image can be digitized and analyzed as an array, with each element resolved into 256 levels of grey. By measuring the standard areas and relating their transmission to the known radioactivities which created them, it is possible to measure any image element in terms of its radioactive content.

This approach of whole body ARG was found to be very useful in the biological evaluation of short-lived positron-emitting radiopharmaceuticals in small laboratory animals, such as mice and rats. Radionuclide distribution in the total body at different times, or under different experimental conditions, is studied conveniently. For example, glucose utilization in normal mice, before and after sedation with chlorpromazine, using fluorine-18-labeled fluorodeoxyglucose (^{18}F-FDG) and carbon-14-labeled-2-deoxyglucose (^{14}C-2DG) revealed a generalized decrease in the glucose utilization, except in the myocardium, under sedation. Furthermore, ARG of sheep brain with ^{18}F-FDG offered excellent delineation (better than that obtained by tomography) of the regional glucose metabolism as identified from the corresponding histological section.

We have been able to show that ^{18}F-FDG concentrates in the brain, heart, and a variety of tumors. The whole body distribution of ^{14}C-2DG in normal mice and mice with transplanted breast adenocarcinoma showed high concentrations in the brain, and viable tumor tissues (Fig. 4). Studies are being conducted to compare and correlate the distribution of old and new tumor-seeking radiopharmaceuticals (viz. ^{67}Ga-citrate, ^{97}Ru-transferrin, ^{3}H-thymidine) using the multiple tracer ARG technique to assess and understand the pathophysiology of different tumors and their response to therapy. Quantitative ARG techniques will also be useful for determining macro- and microscopic radiation dose distributions for newly developed radiopharmaceuticals. ARG is proving to be an increasingly important tool in nuclear medicine radiopharmaceutical and metabolic research.

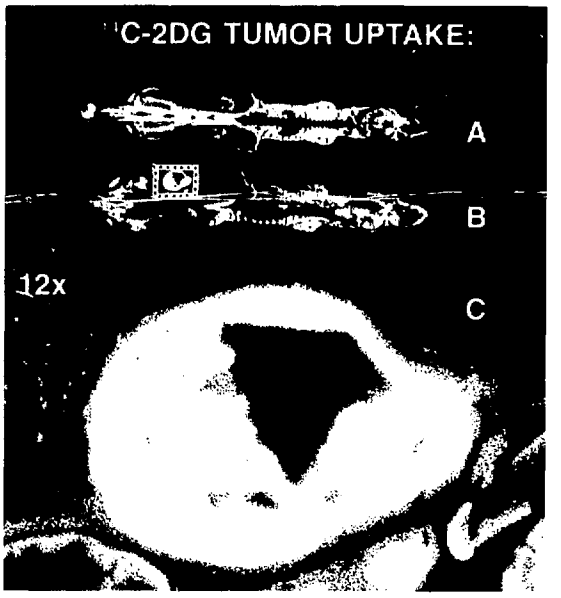

Figure 4. A. Whole body distribution of ^{14}C-2-deoxy-D-glucose (^{14}C-2DG) in normal mouse. B. Same in mouse with transplanted breast adenocarcinoma. C. Enlarged image of tumor shows necrotic center with lack of ^{14}C-2DG uptake, surrounded by viable tissue.

(2) Radiation Therapy of Malignant Melanoma

Iodine-125

Despite encouraging clinical studies showing that irradiation of choroidal melanoma (malignant tumors of the eye), results in survival equal to or better than obtained by surgical removal of the eye, radiation therapy is little

used in most medical institutions for eye tumor therapy. Arguments against the use of the high energy cobalt ^{60}Co plaque ophthalmic applicator, which is the usual irradiator used, include (a) the misconception that melanoma is radioresistant; (b) that the use of the plaque invariably results in severe complications; and (c) the problems of radiation safety and exposure of hospital personnel to high energy gamma rays from ^{60}Co. We know that low energy x-rays, and conversion electrons from ^{125}I are preferable for treating many types of cancer, based upon knowledge of radiobiology and radiation safety considerations. Laboratory evaluations at Brookhaven National Laboratory with ^{125}I and malignant melanoma have led to clinical trials which are now in progress. The ^{125}I is supplied as seeds that are implanted near the tumor. This reduces the radiation exposure and allows for directional radiation when the seeds are placed in plaques.

Initial clinical studies have been with malignant melanomas of the eye. We have treated patients with large intraocular tumors that, were it not for ^{125}I radiotherapy, would have had the eye removed (enucleated). This work was published in 1980 and the technique is now being used with increasing frequency by ophthalmic surgeons and radiation therapists at other medical centers in the United States.

Hyperthermia

Adjuvant therapy in the form of hyperthermia would be desirable. The problem has been lack of appropriate heating devices that could be used clinically. A new hyperthermia-producing device has been designed at Brookhaven that is well-suited for treating cancer in conjunction with the ^{125}I seed radiotherapy. Preliminary laboratory studies have shown this device to be sturdy and able to deliver controlled hyperthermia to animals with tumors.

Hyperthermia along with ionizing radiation acts synergistically in killing cancer cells, including malignant melanoma. The two treatment modalities damage the melanoma cell in different phases of the cell cycle and therefore are complementary forms of therapy. Since melanomas have a long cell cycle, radiation alone has achieved limited success. The ^{125}I radiation partially circumvents this problem by allowing delivery of higher doses of radiation to the tumor for a longer time, thereby irradiating a larger fraction of the cell cycle, while at the same time sparing normal structures. In addition, animal tumor studies show that efficacy is enhanced with hyperthermia.

Future studies will be in *human* melanoma cell lines in mice so that our results with radiation and hyperthermia may more closely resemble the clinical situation, and hopefully, will lead to clinical application. A collaborative effort with the Department of Radiation Oncology at the State University of New York, Downstate Medical Center, is now being pursued.

PROMPT GAMMA NEUTRON ACTIVATION ANALYSIS (PGNAA)

Cadmium

The neutron activation facility for the *in vivo* measurement of cadmium was mounted on a 10.4m mobile trailer unit and (with the support of the International Lead-Zinc Research Organization) was used to monitor levels of cadmium in industrial workers in a smelter at Denver, Colorado, and control subjects. Dose-effect relationships between kidney cadmium burden and kidney damage, as manifested by high urinary levels of β_2-microglobulin, were evaluated in these workers. These important data on the industrially exposed workers provided a basis for determining critical kidney concentrations with respect to biological effect. They are also valuable for setting or revising permissible levels for industrial and environmental cadmium pollution.

Cadmium was measured *in vivo* in the left kidney and liver of 83 industrially exposed workers and 10 control subjects. The range of Cd values for the industrial group was 0.9 – 57 mg for the kidney and 0.8 – 120 ppm for the liver. In the control group, the Cd range was 0.4 – 11.8 mg for the kidney and 0.6 – 7.9 ppm for the liver. In general, the kidney Cd burdens increased with increasing liver concentrations for liver values below 40 ppm. Thereafter, the kidney Cd content decreased as the liver concentration increased. The bi-phasic relationship between kidney Cd and liver Cd would indicate a change occurring at approximately 31 mg for the kidney. Urinary β_2-microglobulin and urinary protein were also used to estimate the critical value for the kidney. The present

study would indicate a range of 31 – 42 mg for the whole kidney (300 – 400 μg/g renal cortex) as the critical level in humans.

Neutron Sources

A comparison was made of the isotopic neutron sources ^{252}Cf and ^{238}Pu,Be for partial body *in vivo* neutron activation analysis. Depth distributions of thermal neutron fluences in a water phantom are very similar for the two sources. The peak depth occurred at 5 cm. This value is approximately 2 cm less than the value obtained with uncollimated neutrons produced in broad-beam irradiation. With respect to the fluence-to-dose ratio, the ^{252}Cf neutrons have an advantage of approximately 1.4 over the ^{238}Pu,Be source.

The use of ^{252}Cf offers two additional advantages for the investigator. First, it minimizes the on-line fast neutron damage in Ge(Li) semiconductor detectors. Secondly, it is subject to much less stringent transport regulations than ^{238}Pu,Be. The latter feature takes on particular importance in view of the increasing usefulness of transportable instruments for *in vivo* cadmium measurements at the workplace.

Nitrogen

A NIH-NCI contract supports a combined BNL-Long Island Jewish-Hillside Medical Center study on *in vivo* quantification of body nitrogen in normal subjects and cancer patients, and on changes in body composition in cancer patients as related to diet. The technique of PGNAA of total body nitrogen (TBN) has been validated and the calibration completed. To date, TBN has been measured in 135 normal male subjects and 60 cancer patients. On the completion of this study, a mathematical model for the determination of the normal levels of nitrogen was developed as a function of age, sex, and the size of the subject. The deficit in TBN was then evaluated in cancer patients.

The techniques of PGNAA for the measurement of total body nitrogen (TBN) and whole body counting for the measurement of total body potassium (TBK) were used to determine the mass of muscle and nonmuscle lean tissue and their protein content in 135 normal male and female subjects, 20-80 yr of age. Age-related changes in the size of the muscle and nonmuscle compartments and their protein content provide basic data for the investigation of protein metabolism in aging subjects and in individuals with various metabolic disorders, particularly wasting diseases such as cancer. Significant age-related changes in the size of various body compartments were noted. The loss of muscle mass and its protein content contrasts with the relative constancy of the nonmuscle lean tissue and suggest that skeletal muscle is particularly vulnerable to the aging process.

The prompt gamma neutron activation and whole body counting techniques represent a considerable advance over the balance and radioisotope techniques used in earlier studies. The new techniques make possible sequential studies of TBN and TBK over prolonged periods of time with a considerable degree of accuracy.

NUCLEAR RESONANT SCATTERING

A technique for the measurement of body iron utilizing nuclear resonant scattering of gamma rays has been developed and validated. From this prototype study, a full scale facility is being developed for clinical application. Photons (847 keV) emitted from a gaseous $^{56}MnCl_2$ source (prepared in the BNL Medical Reactor) are scattered resonantly from ^{56}Fe present in the liver and heart (Fig. 5). The spatial uniformity of activation, the sensitivity of the detection system, and the limits of detection have been investigated. Measurements were made on a liver phantom and two patients. The resonance scattering technique permits detection of normal levels of Fe in the liver with a radiation dose of 2 Rem.

DELAYED GAMMA NEUTRON ACTIVATION ANALYSIS

Physical Therapy

Studies of the effects of physical therapy on the skeletal mass of older human subjects are in progress with the support of an NIH Aging Institute grant. These studies include measurement of the normal changes in skeletal mass with age. The measurement of total body calcium levels in 135 normal subjects, 20-90 years of age, was completed.

Figure 5. Measurement of iron in the heart by nuclear resonance fluorescence.

Combination Therapy

The study of the effects of combination therapy which simultaneously stimulates bone formation and inhibits bone resorption in osteoporotic patients was continued. To date, 50 patients were studied before and after one to two years of growth hormone-calcitonin therapy. The results continue to reinforce the finding of a positive Ca balance previously reported, suggesting an increased skeletal mass after combination therapy.

Skeletal Mass in Patients on Anti-convulsant Therapy

The technique of *in vivo* total body neutron activation analysis was used to measure total body Ca (TBCa), a sensitive and precise index of skeletal mass, expressed as the Ca ratio (TBCa observed/TBCa predicted). Twenty-three unselected, ambulatory, noninstitutionalized, adult epileptic patients under long-term anticonvulsant therapy were studied. The Ca ratio was normal in 20 of the patients, low in only two, and borderline in one patient. Plasma alkaline phosphatase values were elevated in half the subjects. Plasma Ca (uncorrected) was in the normal range for all. Serum 25-hydroxyvitamin D was low in 67% of the subjects.

This study does not support the notion of a prevalence of osteopenia in ambulatory, noninstitutionalized, adult epileptic patients receiving chronic anticonvulsant therapy, despite the frequent findings of biochemical abnormalities.

Total Body Electrolyte Composition and Distribution of Body Water in Uremia

Total body sodium and chlorine were measured by neutron activation analysis, and total body potassium was measured by whole body counting in ten male patients with end-stage renal disease requiring chronic maintenance hemodialysis. The extracellular fluid volume was estimated from the simultaneously measured volume distribution of ^{77}Br and ^{24}Na. Total body water was estimated from the volume distribution of tritiated water. Total body sodium and chlorine were significantly increased above normal measured values, but total body potassium was not significantly different from normal. The increase in total body sodium could be attributed to an increase in exchangeable sodium because no significant change in the nonexchangeable portion of total body sodium could be detected. Extracellular fluid volume, estimated from three different techniques (total body chloride, ^{24}Na, and ^{77}Br), and total body water were increased significantly above normal values. Despite adequate control of uremia by chronic maintenance hemodialysis, body electrolyte composition and the distribution of body water remain significantly different from normal.

Total Body Sodium and Sodium Excess in Post-menopausal Women

Total body levels of sodium (TBNa), chlorine (TBCl), calcium (TBCa), and potassium (TBK) were measured by neutron activation and analysis of results by whole body counting in 66 postmenopausal women. The relationship between TBNa, TBCl, TBK, and TBCa and the parameters of height and weight were found to

compare with those previously reported. The hypothesis that TBNa and TBCl are distributed normally could not be rejected.

The sodium excess (Na_{es}) is defined as the sodium that is present in excess of that associated with the extracellular fluid (chlorine) space; the Na_{es} approximates nonexchangeable bone sodium. In these 66 postmenopausal women, and in patients with different endocrine dysfunctions previously described, the values of Na_{es} did not differ from the normal values except in the thyrotoxicosis patients, where they were decreased.

NEW NUCLEAR TECHNIQUES FOR APPLICATION IN ENVIRONMENTAL HEALTH STUDIES

Silicon and Beryllium Studies

Feasibility studies were initiated for the *in vivo* measurements of silicon and beryllium by nuclear techniques. Silicon, in the form of free crystalline silica, and beryllium, as BeO dust, are potentially hazardous lung contaminants. Silicosis is a chronic fibrosing of the lungs that may occur in workers in a variety of industries including mining, quarrying, and stone cutting. Berylliosis is a granulomatous disease that may develop after even a very brief exposure of an individual to Be or to one of its alloys.

Experiments were performed to measure silicon *in vivo* by means of the prompt neutron inelastic scattering reaction $^{28}Si(n,n'\gamma)^{28}Si$. The optimum neutron energy in terms of counts per dose delivered to a liquid tissue-equivalent phantom was found to be in the range of 5 to 8 MeV, with the use of the Brookhaven RARAF (Van de Graaff) facility.

When the neutron beam was pulsed and counting performed only in the "on" period, it was possible to reduce substantially the background both from thermal neutron interactions in the phantom and those from the fast neutron interfering reaction $^{31}P(n, \alpha)^{28}Al$. In measurements with a realistic chest phantom, no interferences from other prompt inelastic scattering reactions were observed. With one Ge(Li) detector of 19% relative efficiency, a detection limit of 0.6 g silicon per Rem was obtained. A system comprised of six 25% efficient detectors should be capable of measuring normal lung silicon contents of about 0.1 g.

These experiments demonstrate the feasibility of measuring silicon *in vivo* by the method of prompt neutron inelastic scattered gamma ray analysis. A practical system based on the use of 5-8 MeV neutrons from a pulsed Van de Graaff accelerator would be capable of detecting normal lung contents of about 0.1 g silicon with a dose of 1 Rem. For screening workers suspected of suffering from silicosis, useful data might be obtained with doses of less than 0.1 Rem.

The problems associated with the determination of levels of beryllium contamination are more complex than those encountered with silicon, as the quantities involved are smaller. Berylliosis has been observed in persons with lung contents ranging from micrograms to tens of milligrams (a normal value is 1-2 μg). While there is evidence that the human response to this contamination contains a distinct immunological component, and individual hypersensitivity is important, a recent study found a dose-response relationship for some workers. *In vivo* measurements are useful for the latter individuals.

The use of the uniquely low photonuclear threshold of Be has been considered. Photons of energies between 1.665 and 2.225 MeV (deuterium γ, n threshold) would be used for irradiation, and the neutrons produced would be counted. It has been calculated that for a monoenergetic photon source of about 1.7 MeV, it should be possible (depending on the detection efficiency) to measure lung contents of fractions of a milligram with an associated dose of several rads. On the basis of results with a 50 mCi, Pb-filtered ^{124}Sb source and enriched $^{10}BF_3$ counters, the construction of a larger facility to examine the detection response at realistic dose rates of several rads/h has been recommended.

Lead Studies

Preliminary measurements of lead content of bone tissue was performed with x-ray fluorescence. In contrast to the technique developed by the Swedish group which utilizes the measurement of the 75 keV K x-ray, it is proposed to measure the characteristic L x-ray of lead (10.5 keV) emitted from bone surfaces of a finger or the tibia. Although the L x-rays have a lower probability of escaping from the tissue, the cross-section for their production (with a source with suitable energy) is considerably higher.

Lead deposits in bone were detected by x-ray fluorescence with the use of x-rays from either a ^{125}I or a ^{109}Cd source. Measurements were taken from tibias of five intact human legs, post-mortem. On the basis of preliminary measurements, it was concluded that an exposure of 1 rad is adequate for determination of lead in bone. The study demonstrates that L-x-ray fluorescence can be used for the *in vivo* measurement of lead concentration in the tibia. The higher polarizability of the incident radiation at lower energies may improve the overall performance of the system. A study is under way to correlate the strontium peak with the calcium content of the sampled mass of the bone. This technique may be advantageous in normalizing the measured lead intensities. Presently the detection limit for lead is estimated to be between 10 and 20 ppm. A more precise value for the detection limit will be determined later. The reproducibility of the system, as estimated from measurements of the strontium peak, is about ±10%.

RADIONUCLIDE RESEARCH PROGRAM

This program covers many different aspects of radiopharmaceutical research leading to new and improved diagnostic and therapeutic agents, with particular emphasis on disease resulting from, or aggravated by, energy-related pollutants. The research involves extensive collaboration with off-site research groups, and utilizes many unique Laboratory facilities including the BLIP (Brookhaven Linac Isotope Producer), HFBR (High Flux Beam Reactor), high-level radiation processing cells, and the excellent veterinary and clinical facilities. The significant impact of the BLIP and its continuing usefulness to the nuclear medicine community has been amply demonstrated during the past several years. The BLIP continues to be a unique source for efficient and economical production of difficult to produce medically useful radionuclides for on-site research programs as well as for a number of outside collaborative programs.

The major objective of this program, like those of the more comprehensive Nuclear Medicine Program of which it is an integral part, is to perform research leading to improvements in the quality of health care provided by the medical profession. The program is aimed at carrying out research on the design and application of new and improved radiopharmaceuticals based on potential radionuclides. Past and continuing achievement of these goals is evidenced by the development of technetium-99*m*, technetium-99*m*-radiopharmaceuticals, thallium-201, ruthenium-97, and the present increasing demand for xenon-127. Currently, over 80% of all diagnostic nuclear medicine procedures involve one of these radionuclides. The scope of this program is broad, covering all aspects ranging from selection and development of the starting material to the final clinical evaluation of promising radiopharmaceuticals.

The long-range objectives are: A. To design and develop new or improved radiopharmaceuticals that would (1) lead to better understanding of physiological processes, (2) provide improved methods of diagnosis in nuclear medicine procedures, and (3) impart reduced radiation dose to the patient; B. To elucidate the mechanisms involved in the biodistribution and tissue uptake of selected radiopharmaceuticals; C. To evaluate and establish the potential of a large high-energy particle accelerator for efficient and economic production of medically useful nuclides and devise the technology by which industry can make them available to the public; and D. To provide research quantities of new and/or otherwise difficult to produce radionuclides to the nuclear medicine community. Extensive chemical studies, development of sensitive analytical procedures, animal evaluation, mechanistic investigations, and preliminary clinical trials are integral parts of this program.

During the past year BLIP again demonstrated the capability to have a significant impact on the medical community as a resource for difficult to produce medical radionuclides. Several radionuclides were distributed routinely to industry and medical institutions, including ^{109}Cd, ^{68}Ge, and ^{127}Xe. The latter played an important role in the BNL pulmonary program. A number of other radionuclides were produced for research collaborators as well as for the BNL nuclear medicine research program, e.g., ^{123}I, ^{52}Fe, and ^{97}Ru. Several others are under development; ^{128}Cs, ^{178}Ta, and ^{191m}Ir, which could prove to be important biomedical tracers.

Work continued on a collaborative program with Columbia College of Physicians and Surgeons on a technique for the synergistic suppression of the body's immune response following organ transplants by the use of ^{109}Pd-labeled hematoporphyrin in conjunction with anti-lymphocyte serum.

The areas of major emphasis during the past year were: A. development and evaluation of new radiopharmaceuticals based on ^{97}Ru; B. labeling of blood cells (erythrocytes, leukocytes, and platelets) with ruthenium, technetium, and tin radionuclides, and C. the chemistry and analysis of tin-technetium radiopharmaceuticals. *In vivo* experiments in mice, rats, and dogs demonstrated considerable promise for clinical usefulness of a number of ^{97}Ru-labeled compounds: transferrin (tumor-localization); iminodiacetate derivatives (hepatobiliary agents); dimercaptosuccinic acid (kidney studies); diethylenetriamine pentaacetic acid (DTPA) (cisternography); and oxine and acetylacetone derivatives (labeled blood cells), etc.

Growth in the use of radionuclide procedures in cardiology has continued at a rapid pace and created an increasing demand for ^{99m}Tc-labeled red blood cells (RBC) because they are considered ideal for assessing damage to ventricular function following myocardial infarcts. The BNL RBC-labeling kit, developed earlier in this program, is finding widespread use for these applications. The kits are being distributed to forty medical institutions in the US and abroad. The mechanism of this labeling reaction is under investigation; several important findings were uncovered recently, for example that the technetium binds preferentially to the beta globin chain of the hemoglobin molecule, and that the binding reaction is affected by the presence in blood of the RBC antibodies in patients undergoing therapy with certain types of drugs. These results may have clinically useful implications. A recent modification in the BNL RBC kit has extended its usefulness to the diagnosis of splenic disorders in infants and children.

The powerful new technique of high-performance liquid chromatography (HPLC) has been applied to the analysis of ^{99m}Tc radiopharmaceuticals (Fig. 6). It was demonstrated that many clinically used ^{99m}Tc imaging agents are complex mixtures, and not single well-defined compounds, as commonly believed on the basis of results from routine quality control methods. This highly sensitive technique offers renewed prospects for a better understanding of the chemistry and the localization mechanisms of technetium radiopharmaceuticals. This much needed information is required for the development of new and more efficacious compounds for obtaining reliable clinical data, as well as for improvements in the existing agents.

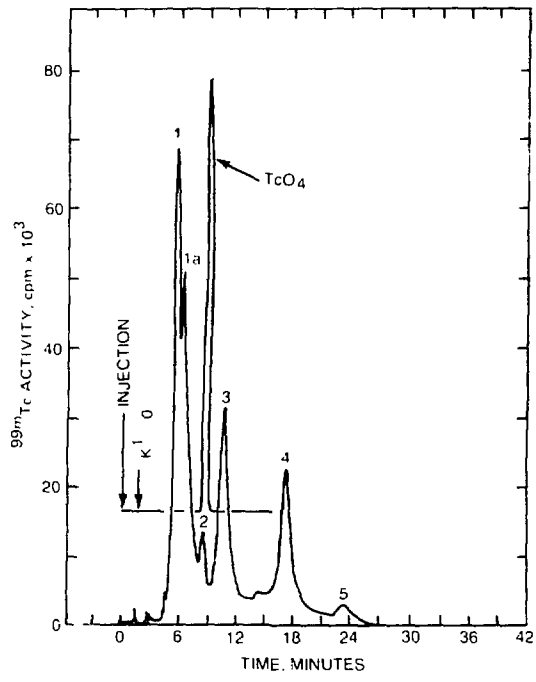

Figure 6. A typical HPLC (high performance liquid chromatography) analysis of a clinically used bone-imaging agent, technetium-99*m*-labeled methylenediphosphonate (^{99m}Tc-MDP). Note that the preparation contains multiple components, and not a single homogeneous compound, as believed earlier, based on results of routine quality assurance methods. Elution pattern of the starting material (pertechnetate, $^{99m}TcO_4^-$) is included for comparison with that of the final labeled product (peaks 1 – 5). Detection and quantitation of pertechnetate as a radiochemical contaminant in the final preparation is readily possible with this technique. A variety of detection modes can be utilized for the various species; in this experiment, gamma radioactivity (resulting from ^{99m}Tc) detection was employed.

Selected Publications

G. W. BENNETT, A. B. BRILL, R. G. FAIRCHILD, R. S. DOBERT, A. T. POKROPEK, M. SHORT, P. ESSER, AND M. K. ZAIDI, A multi-purpose phantom for gated, computer-aided gamma camera studies. IAEA/SM-247/101. *IAEA International Symposium on Medical Radionuclide Imaging, Heidelberg, Germany, Sept. 1-5, 1980* (in press).

A. B. BRILL, National Research Council, Committee on Biological Effects of Ionizing Radiation (BEIR). *The Effects on Populations of Exposure to Low Levels of Ionizing Radiation: 1980,* National Academy Press, Washington, DC, 1980, pp. 331-57.

S. PACKER, M. ROTMAN, R. G. FAIRCHILD, D. M. ALBERT, H. L. ATKINS, AND B. CHAN, Irradiation of choroidal melanoma with iodine-125 ophthalmic plaques. *Arch. Ophthalmol.* **98,** 1453-57 (1980).

R. A. CONARD, Review of Medical Findings in a Marshallese Population Twenty-Six Years After Accidental Exposure to Radioactive Fallout (in preparation).

R. T. DREW, "The development of the standard inhalation chamber," in *Inhalation Chamber Toxicology,* BNL Report 51318 (in press).

D. M. BERNSTEIN, R. T. DREW, AND M. KUSCHNER, The deposition, translocation, and fate of sized man-made fibers in rats. *Third Annual Report to Thermal Insulation Manufacturer's Association,* Mt. Kisco, New York (BNL Information Report No. 28994) (1980).

J. IWAI, R. FRIEDMAN, AND L. TASSINARI, Genetic influence on brain catecholamines: high brain norepinephrine in salt-sensitive rats. *Clin. Sci.* **59,** 263s-265s (1980).

S. H. COHN, A. SAWITSKY, D. VARTSKY, S. YASUMURA, I. ZANZI, AND K. J. ELLIS, *In vivo* quantification of body nitrogen and body composition in normal subjects and in cancer patients for cancer nutrition studies. *Nutr. & Cancer, Int. J.* **2,** 67 (1980).

S. H. COHN, D. VARTSKY, S. YASUMURA, I. ZANZI, AND K. J. ELLIS, Critical concentrations of cadmium in human liver and kidney measured by prompt-gamma neutron activation. *Cadmium* **79,** 168 (1980).

S. H. COHN, The present status of *in vivo* neutron activation analysis in clinical diagnosis and therapy. *Atomic Energy Review,* IAEA, Vienna, **18,** (No 3), (1980).

S. H. COHN, D. VARTSKY, S. YASUMURA, A. SAWITSKY, I. ZANZI, A. VASWANI, AND K. J. ELLIS, Compartmental body composition based on total body nitrogen, potassium, and calcium. *Am. J. Physiol.* **239,** E524 (1980).

S. C. SRIVASTAVA, P. RICHARDS, P. SOM, G. E. MEINKEN, H. L. ATKINS, A. SEWATKAR, AND T. H. KU, "10 Ruthenium-97 labeled compounds—a new class of radiopharmaceuticals." *Frontiers in Nuclear Medicine,* Springer Verlag, Heidelberg, 1980, pp. 123-133.

J. P. STONE, S. HOLTZMAN, AND C. J. SHELLABARGER, Synergistic interactions of various doses of diethylstilbestrol and x irradiation on mammary neoplasia in female ACI rats. *Cancer Res.* **40,** 3966-72 (1980).

C. J. SHELLABARGER, B. MCKNIGHT, J. P. STONE, AND S. HOLTZMAN, Interaction of dimethylbenzanthracene and diethylstilbestrol on mammary adenocarcinoma formation in female ACI rats. *Cancer Res.* **40,** 1808-11 (1980).

J. SILVERMAN, C. J. SHELLABARGER, S. HOLTZMAN, J. P. STONE, AND J. H. WEISBURGER, Effect of dietary fat on x-ray induced mammary cancer in Sprague-Dawley rats. *J. Natl. Cancer Inst.* **64,** 631-34 (1980).

A. L. CARSTEN, "History and overview of the *in vivo* diffusion chamber (DC) culture system" in: *Diffusion Chamber Culture—Hemopoiesis, Cloning of Tumors, Cytogenetic and Carcinogenic Assays,* E. P. Cronkite and A. L. Carsten, Eds., Springer Verlag, Heidelberg, 1980, pp. 3-11.

A. D. CHANANA, P. CHANDRA, AND D. D. JOEL, Pulmonary mononuclear cells: Studies of pulmonary lymph and bronchoalveolar cells of sheep. *J. Reticuloendothel. Soc.* **29,** 127-35 (1980).

S. L. COMMERFORD, V. P. BOND, AND E. P. CRONKITE, Radiotoxicity of Intranuclear ^{125}I Atoms not Bound to DNA. *Int. J. Radiat. Biol.* **37** (No. 5), 547-54 (1980).

D. D. JOEL, A. D. CHANANA, AND P. CHANDRA, Immune responses in pulmonary lymph of sheep after intrabronchial administration of heterologous erythrocytes. *Am. Rev. Respir. Dis.* **122,** 925-32 (1980).

M. E. LEFEVRE, D. D. JOEL, AND D. C. HANCOCK, The intestinal barrier to large particulates in mice. *J. Tox. Environ. Health* **6,** 691-704 (1980).

K. HARIGAYA, M. E. MILLER, G. MOCCIA, AND E. P. CRONKITE, Further evidence of the *in vivo* role of erythropoietin or companion molecules induced by hypoxia on proliferation and continuing differentiation of BFU-E in PCDC. *Blood* **57,** 298-304 (1981).

D. C. BORG, K. M. SCHAICH, AND J. J. ELMORE, JR., "Autoxidation and cytotoxicity" in *Oxygen and Oxyradicals in Chemistry and Biology,* M. A. J. Rodgers and E. L. Powers, Eds., Academic Press, New York, 1981 (in press).

K. M. SCHAICH, AND D. C. BORG, "EPR studies in autoxidations" in *Autoxidation in Foods and Related Biological Systems,* M. Simic and M. Karel, Eds., Plenum Press, New York, 1980, pp. 45-70.

W. LAUTERBURG, R. D. STONER, H. COTTIER, B. RYFFEL, H. BUERKI, AND M. W. HESS, Increased lymphocyte load of postcapillary venules in regional lymph nodes following stimulation with antigen-isologous antibody complexes as compared with antigen alone. *Blood Cells* **6,** 41-51 (1980).

MEDICAL DEPARTMENT

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R. B. Aronson, Deputy Chairman

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R. T. Drew, Coordinator

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Interrelationships Among Genetic Factors and Environmental Pollutants in Clinical and Experimental Hypertension — **J. Iwai, S. B. Haber, R. Friedman.**

Inhalation Toxicity of Glass Fibers (TIMA) — **R. T. Drew.**

Respiratory Pathology Training Grant (NIEHS) — **R. T. Drew, R. N. Shiotsuka.**

Inbreeding of Dahl S and R rats (NHLBDI) — **J. Iwai, S. B. Haber.**

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Diet, Nutrition, and Cancer (NCI) — **S. H. Cohn, A. N. Vaswani, D. Vartsky.**

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Oxidative and Free Radical Mechanisms Involved in the Cytotoxicity and Carcinogenicity/Mutagenicity of Pollutants — **D. C. Borg, J. J. Elmore, A. Forman, K. M. Schaich, S. N. Rosenthal.**

Interaction Between Energy-Related Pollutants and Oncogenic Viruses in Carcinogenisis — **M. T. Pavlova.**

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Connective Tissue Metabolism — **E. A. Popenoe.**

Training Workshops in Detection of Environmental Mutagens, Carcinogens, and Teratogens — **A. Hollaender, R. R. Tice.**

Evaluation of Hazards of By-Products from Nuclear and Non-nuclear Energy Generation — **A. L. Carsten, R. D. Benz, S. L. Commerford, D. N. Slatkin.**

Human Chromosomal Aberration Production by Energy-Related Agents — **M. A. Bender, R. R. Tice, R. Kale, J. Wieland.**

Teratogenesis — **D. W. Slater.**

Effects of Dose Rate on Rat Mammary Carcinogenesis — **C. J. Shellabarger, V. P. Bond, E. P. Cronkite.**

Chemoprevention of Epithelial Cancer by Retinoids — **C. J. Shellabarger, J. P. Stone, S. Holtzman.**

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Effects of Chemicals and Radiation on Control of Hemopoiesis — **E. P. Cronkite, H. Burlington, A. D. Chanana, S. L. Commerford, D. D. Joel, J. E. T. Kelley, M. E. Miller.**

Measurement of Cell Death in Animals Chronically Exposed to Toxic Agents — **S. L. Commerford.**

The Detection of Residual Injury by Pollutants and Rapid Testing for Leukemogenesis — **E. P. Cronkite, G. E. Hubner.**

Penetration through the Gut and Bioeffects of Particulates from Nonnuclear Energy Production — **D. D. Joel, M. E. LeFevre.**

Early and Late Effects of Energy-Related Pollutants on Immunologic Systems — **R. D. Stoner.**

Regulatory Mechanisms of Erythropoietin Production (NHLBDI) — **M. E. Miller.**

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Applied Energy Science

Department of Energy and Environment

Department of Nuclear Energy

Department of Energy and Environment

INTRODUCTION

The objectives of the Department of Energy and Environment (DEE) are to generate a base of scientific, economic, and technical data on selected energy technologies and on the effects of energy-related activities on the environment. The research and development in the fundamental and applied program is performed in four main areas (1) Energy Sciences, (2) Environmental Sciences, (3) Energy Technology, and (4) The National Center for Analysis of Energy Systems.

Energy Sciences

CHEMISTRY, MATERIALS, AND PROCESS SCIENCES PROGRAMS

In the area of Energy Sciences work is carried out in the chemical, materials, and process sciences. The chemistry studies are concerned with basic and applied research on synthetic photosynthetic compounds, combustion of fuels, mechanisms involved in coal liquefaction, analytical methods, studies of membranes, metal hydrides, and other related studies.

Research on materials is focused on the study of materials of importance in the production, transmission, and storage of energy. Included are studies of superconducting materials, hydrogen in metals, materials for dielectrics in power transmission cables, electrode materials, and behavior of materials under stress and in corrosive media.

The work in process sciences applies chemical and physical methods and techniques to the development of efficient and environmentally acceptable processes for the conversion of natural resources to the production of fuel, power, and materials of construction to meet energy requirements in the U.S.

Recent advances during 1980 in the Energy Sciences are reported below.

CHEMICAL SCIENCES DIVISION

Kinetics and Mechanisms of Alternative Fuels Combustion

Two complementary experimental techniques to obtain direct, absolute rate data for combustion-related elementary reactions over a wide range in temperature (nominally 350-1100 K) were successfully carried out.

One set of reactions investigated involved a series of low molecular weight hydrocarbons in which the specific reaction studied was that of an oxygen atom abstracting a hydrogen atom, viz.,

$$O + R{-}\underset{\displaystyle H}{\overset{\displaystyle H}{\overset{|}{\underset{|}{C}}}}{-}H \xrightarrow{k} R{-}\underset{\displaystyle H}{\overset{\displaystyle H}{\overset{|}{\underset{|}{C}}}}\cdot + OH\cdot$$

Expressing the specific rate constant, k, in Arrhenius form

$$k = Ae^{-E_a/RT}$$

the kinetic results of this investigation are summarized in Table I.

Table I. Hydrocarbon Oxidation Rate Constants

Hydrocarbon	R	C-H Bond Energy (kcal mole^{-1})	A x 10^{10} (cm^{3}sec^{-1})	E_a (kcal/mole^{-1})
Methane	H	104.2	2.1	10.5
Ethane	CH_3	98.8	1.9	7.8
Propane	CH_3CH_2	94.5	1.8	6.4
Iso-butane	$H_3C-\underset{\displaystyle CH_3}{\overset{\displaystyle CH_3}{\overset{\displaystyle |}{\underset{\displaystyle |}{C}}}}$	92.7	1.5	5.5

The correlation between the activation energy (E_a) and the C-H bond energy is at once apparent and is as expected. The apparent general trend toward lower collision factor (A) values in the series has as yet no detailed theoretical explanation.

The discrepancy between these data and previously reported results appears to lie in the fact that older experiments had to be performed at considerably higher atom and radical concentrations, due to the relatively low detection sensitivity then available. These higher concentrations resulted in significant secondary reactions, which had to be corrected for. The data obtained in this investigation were obtained in a regime of concentration where secondary reactions were minimized and did not have to be considered.

In another investigation — that of hydrogen atom abstraction from methanol (CH_3OH) by oxygen atoms — good experimental agreement was obtained with a recent, concurrent investigation elsewhere. Both sets of experimental results are in disagreement with those of earlier investigations. In this case, too, much of the discrepancy can be attributed to the higher atomic oxygen concentrations necessitated in the earlier investigations.

On the Non-Ideal Behavior of Certain Metal Alloy-Hydrogen Systems

It has been observed that dilute solutions of hydrogen in certain intermetallic compounds deviate markedly from ideal behavior, i.e., they do not obey Sievert's law. The most striking feature of the deviation is that it becomes more pronounced as the hydrogen concentration approaches zero as illustrated in Fig. 1. This behavior has been found to be common to all dilute inter-metallic-hydrogen systems in which the two metal components are an exothermic and an endothermic dissolver of hydrogen, e.g., $LaNi_5$, $TiCr_{1.8}$, and FeTi. The original question posed was whether these systems are truly non-ideal, perhaps as a result of H-H repulsion, or is their unusual behavior due to experimental artifacts or defects common in intermetallic compounds. Evidence in the literature for

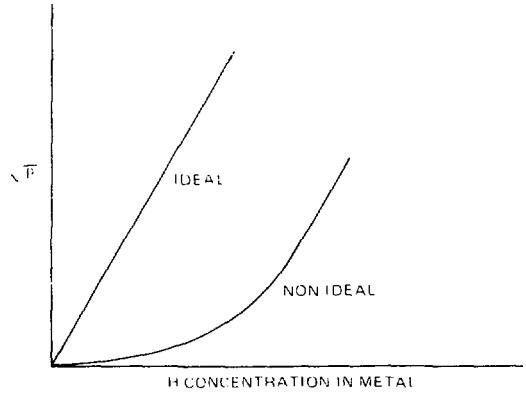

Figure 1. Sievert's plot showing the concentration of hydrogen in a metal as a function of $\sqrt{P}$. P is the equilibrium pressure of hydrogen in the gas phase. The square root dependence arises from the fact that the hydrogen molecules dissociate into atoms upon dissolving in the metal.

$LaNi_5$ suggested the latter possibility was most tenable. Such defects could be homogeneously distributed throughout the bulk of the material or could be localized, e.g., in surface layers produced by surface segregation effects.

We undertook to distinguish between these possibilities in the FeTi-H system using x-ray diffraction, exploiting for this purpose the fact that the rate of lattice expansion as a function of hydrogen content is a constant for all transition metals and alloys in the solid solution region.

As a result of this study we have concluded that the non-ideal behavior of cubic $FeTiH_x$ in the solid solution region is due to two causes; segregation of hydrogen in three-dimensional surface phases produced by surface segregation effects and, with activated (previously hydrided-dehydrided), non-annealed samples, trapping of hydrogen in bulk defects produced by the cold work incurred during the activation process. Thus the observed deviations are not due to any inherent system property but merely to experimental artifacts and the presence of bulk defects produced by the activation pretreatment step. These conclusions are supported by recent work by the Jülich group which, using a thermodynamic approach, has shown that, when surface and cold work effects are eliminated, the cubic $FeTiH_x$ system behaves ideally throughout the entire solid solution region.

We are similarly investigating the $LaNi_5H_x$ system in the dilute solid solution region. We have concluded that in this system hydrogen segregation is not a contributory cause of the observed deviant behavior. Preliminary results indicate that bulk defects resulting from the activation process and/or non-stoichiometry are solely responsible.

For the intermetallic compound $TiCr_{1.8}$ the apparent departure from ideal behavior is correlated to the inherent non-stoichiometric character of this material and is most likely due to dual site occupation by hydrogen.

METALLURGY AND MATERIALS SCIENCE DIVISION

Superconducting Materials

Applications of superconductivity will find an increasing role in the energy technology of the future; superconducting power transmission lines and the use of superconducting magnets for thermonuclear devices and accelerators are examples. Our research has focused on the properties of a number of superconducting compounds with the *A*15 crystal structure (e.g., Nb_3Sn, V_3Ga, V_3Si, etc.), their behavior as elements of simple composite conductors, and on novel methods for fabricating such composite conductors.

Recently we have studied how the superconducting critical properties of *A*15 compounds vary with elastic deformation of the lattice shape and volume[1,2], and how this strain dependence is affected by alloying additions[3] and lattice disorder produced by neutron irradiation.[4] Such strain effects are important because of the presence of stresses due to the Lorentz force during magnet operation. We find that replacing some of the Nb in Nb_3Sn by other transition elements (such as Ta, Mo, Zr, Hf, etc.) produces substantial variations in the strain dependence, often increasing it, and that lattice disorder produced by radiation and strain act synergistically in depressing the critical properties of Nb_3Sn.

We have found a correlation between the temperature dependence of the elastic moduli and the nonhydrostatic strain dependence of the critical properties. For example, decreasing temperature results in an increase of the Young's modulus, E, of V_3Ge and nonhydrostatic strain increases its critical temperature, T_c. However, replacing some of the Ge with Al reverses the sign of both effects. In some cases (e.g., Nb_3Sn, V_3Si) the softening of the elastic moduli leads to a martensitic phase transition. We have explored the temperature dependence of the complex elastic modulus in the vicinity of the phase transition in Nb_3Sn and below the transition temperature found previously undetected internal friction which we attribute to the stress-induced motion of domain walls.

References

1. D. O. WELCH. "Alteration of the superconducting properties of A15 compounds and elementary composite superconductors by nonhydrostatic strain." *Advances in Cryogenic Engineering*, A. F. Clark and R. P. Reed, Editors, Vol. **26** (Materials), pp. 48-65, Plenum, New York (1981).

2. T. LUHMAN and D. O. WELCH. "Studies of strain-dependent properties of A15 filamentary con-

ductors at Brookhaven National Laboratory." *Filamentary A15 Superconductors*, M. Suenaga and A. F. Clark, Editors, pp. 171-86, Plenum, New York (1980).

3. M. SUENAGA, K. AIHARA, and D. O. WELCH. Effects of Ta on the strain dependence of Tc and Hc_2 in A15 $(Nb_1Ta)_3Sn$. *Bull. Am. Phys. Soc.* **25,** 385 (1980).

4. C. L. SNEAD, JR. and M. SUENAGA. Synergism between strain and neutron irradiation in filamentary Nb_3Sn conductors. *Appl. Phys. Lett.* **37,** 659-61 (1980).

Mechanical Properties of Materials

The technologies of energy generation and conversion often subject materials to severe conditions. Thus, considerable research into the mechanical properties of materials at high stress and temperature is necessary to assist in the design of safe and economical energy-generating installations.

The purpose of our research is to determine the relationship between the microstructures of materials and their fracture toughness (a property characterizing the resistance of a material to the propagation of cracks in it). In the past, little effort has been devoted to studying the effect of in-service mechanical damage to materials, such as deformation at constant stress at high temperatures (creep) or deformation by cyclic stresses (fatigue), on their fracture toughness; creep or fatigue may lead to a dangerous reduction of the resistance of the material to the extension of sharp cracks well before the life of the material, as determined from creep or fatigue considerations, has been exceeded.

Recently we have studied the effects of combined fatigue and creep damage on the fracture toughness of Inconel X-750,[1] a nickel-base precipitation hardening alloy widely used as a heat- and corrosion-resistant structural material in energy-generating systems, whose microstructure is shown in Fig. 2.

We examined the effect on the fracture toughness of this alloy of loading with various stress vs time profiles and the effect of introducing holding periods at constant stress. It was found that a period of tensile creep was the most important factor in altering the fracture toughness and other properties. The reduction in fracture toughness after "tensile-hold" fatigue at the end of the fatigue life was typically more than 40%. Studies by electron microscopy

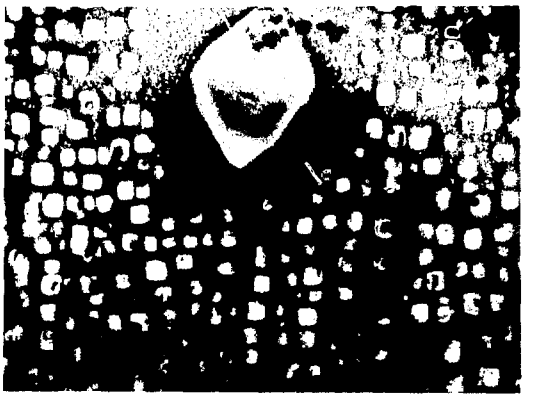

Figure 2. The microstructure of undeformed Inconel X-750 consists principally of precipitates of an ordered intermetallic phase (γ'), which is essentially of composition Ni_3Al, in a nickel-rich solid-solution matrix. The large, square, white particles (~ 1000 Å in size) and the fine white particles are both γ' precipitates, while the large rhombus-shaped particle is an MC-type carbide inclusion.

showed that the introduction of a tensile creep component to the loading profile markedly affected the dislocation morphology and the mode of plastic flow, as well as changing the site of crack initiation from the surface to grain boundaries within the material. These observations suggest that current design codes based on fatigue life or rupture life alone may not be sufficiently conservative in nature.

Reference

1. S. K. HWANG, The Effect of High Temperature Fatigue on the Fracture Toughness of an Inconel X-750 Alloy, *Scripta Met.* (in press).

Materials for Solar Energy

In recent years there has been a worldwide upsurge of interest in amorphous semiconductors; such materials are interesting subjects for study in their own right, and they appear to be promising materials for low cost electronic devices and solar cells.

Thin films of hydrogenated amorphous silicon, a-Si:H, were prepared by the decomposition of silane gas (SiH_4) in a radio-frequency discharge. The film growth process itself has been studied. Optical Emission Spectroscopy (OES), in combination with mass-spectrometric measurements, has revealed the presence of monochlorosilane, SiH_3Cl, as an impurity. The

chlorine, when incorporated into the films, has been shown to act as a p-type dopant. OES has also been used to measure the relative amounts of certain molecular species in the plasma as a function of rf power input, thus giving information on the chemical reaction mechanisms involved in the discharge.[1]

The photoconductive and photoluminescent properties of thin films of essentially "pure" and doped a-Si:H have been studied. Measurements of the photoconductivity of "pure" films as a function of temperature have revealed structure ("peaks" and "valleys") not previously reported in similar measurements elsewhere. We believe that the unusual temperature dependence of photoconductivity is a characteristic of the "intrinsic", or undoped, a-Si:H alloys.[2-4] By contrast, the addition of as little as 1 ppm phosphine gas, PH_3, to the silane in the discharge results in electronically doped n-type films. The room temperature photoconductivity of such films increases by 4-5 orders of magnitude, and the peaks and valleys disappear. The introduction of air or nitric oxide (NO) results in similar n-type doped films, whereas the introduction of either nitrogen or oxygen alone, has no such effect.

In the course of the photoconductivity studies, it was shown that the photo-response can be quenched by infrared light. This effect was used to study the states lying in the mobility gap between the valence and conduction bands, particularly those states which affect carrier recombination and trapping.[5]

Infrared absorption spectroscopy has been used to estimate the amount and bonding of a configuration of hydrogen. We find that the number of $Si\text{-}H_2$ groups and $(SiH_2)_n$ chains, while generally small, increases with increasing rf power and pressure in the discharge.

References

1. F. J. KAMPAS and R. W. GRIFFITH, Origin of Emitting Species in the Plasma Deposition of a-Si:H Alloys, *J. Appl. Phys.* (in press).

2. R. W. GRIFFITH, F. J. KAMPUS, P. E. VANIER and M. D. HIRSCH, Study of Gap States in Low Impurity a-Si:H by Infrared Quenching of Photoconductivity. *J. Non-Cryst. Solids* **35/36,** 391-396 (1980).

3. P. E. VANIER, A. E. DELAHOY and R. W. GRIFFITH, New Features of the Temperature Dependence of Photoconductivity in Plasma-Deposited a-Si:H Alloys, BNL-28833.

4. R. W. GRIFFITH, "Introduction to Basic Aspects of Plasma-Deposited Amorphous Semiconductor Alloys in Photovoltaic Conversion," *Solar Materials Science,* L. E. Murr, Editor, Chapt. 19, pp. 665-731, Academic Press, New York (1980).

5. P. E. VANIER and R. W. GRIFFITH, Modification in Optoelectronic Behavior of Plasma-Deposited Amorphous Semiconductor Alloys Via Impurity Incorporation. *Bull. Amer. Phys. Soc.* **25,** 330 (1980).

PROCESS SCIENCE DIVISION

Calcium Silicate Cements for Desulfurization of Combustion Gases

Commercial silicate cement (Portland Cement Type III) has been found to be a highly effective sorbent for removal of sulfur dioxide under conditions for the fluidized bed combustion (FBC) of coal. The sulfated cement can be regenerated to recover the sulfur dioxide and the sorbent can be recycled for reuse.[1] See section on Sulfur Removal from Hot Gases in Energy Technology Programs.

Ethylene Polymer Conservation

Several pounds of ethylene-sulfur dioxide copolymer have been produced with Co-60 gamma radiation and electron beam radiation at very high yields. The polymer contains up to 70% sulfur dioxide and is thermally stable to 350°C. Methods for forming the material into engineering plastics are being investigated. The material has potential in reducing ethylene consumption in bulk polymers and converting a waste pollutant (SO_2) into a useful product.[2]

Environmental Control Technology for Atmospheric CO_2

Methods for removal and disposal of CO_2 to prevent atmospheric buildup due to the use of fossil fuels which may result in catastrophic climatic effects (greenhouse effect) have been studied. Removal of CO_2 from the atmosphere is energetically not feasible with a fossil-fueled power source. More CO_2 would be generated than removed; however, removal of CO_2 from fossil-fueled power plant stacks is feasible with deep ocean disposal, but severe efficiency and economic penalties would be incurred.[3] A study of the use of cultivated forest planting adjacent to a coal burning power plant in controlling CO_2 emissions has indicated only a marginal value compared to general forestation on a global scale.

Materials for Geothermal Energy Processes

In order to economically develop geothermal resources for energy production, low-cost corrosion-resistant materials of construction are needed.[5] Development work on materials[6] for seals, pumps, well cements, drill bits, casing, piping and heat exchangers is performed in cooperation with universities, private industry and with foreign countries (Iceland, Italy, Mexico and New Zealand).

Long-term testing of materials is under way at many U.S. and foreign geothermal sites. Based upon the results from laboratory and field tests and economic studies performed concurrent with the research, near-term uses in electric generation and space heating appear practical. In addition to use in geothermal processes, this work has already resulted in improved materials for use in the drilling and operation of deep oil and gas wells and in enhanced oil-recovery processes.

Materials for Transportation Applications

The process division is developing materials which can be used for new construction and for rapid repair materials in a variety of transportation systems. Two applications currently being addressed are for bridge decks and for the rapid repair of airport runways.

Under contract to the Federal Highway Administration, BNL has developed polymer concrete patching and bridge deck overlay materials that have the premix characteristics of Portland cement concrete but with superior strength and durability properties.[7,8] Evaluation of the materials by several state transportation departments is in progress.

References

1. A. ALBANESE, D. SETHI and M. STEINBERG. Regenerative Portland Cement Sorbents for Fluidized Bed Combustion of Coal. BNL 27840, May 1980.

2. M. STEINBERG, R. JOHNSON, D. ELLERY, P. BERNSTEIN, and A. VARKER. Polysulfones for Conservation in the Ethylene Polymer Industry, Status Report. BNL 27864, April 1980.

3. M. STEINBERG and A. S. ALBANESE, Environmental Control Technology for Atmospheric Carbon Dioxide. Presented at the International Workshop in Energy/Climate Interactions, Munster, March 3-7, 1980 (in press) and BNL 27164, January 1980.

4. V. D. DANG and M. STEINBERG. The Value of Forestation in Absorbing Carbon Dioxide Surrounding a Coal Fired Power Plant, BNL 51279, August 1980.

5. T. E. GASS, W. H. PURDIN, and D. M. ARMITAGE. Economic impact of using nonmetallic materials in low to intermediate temperature geothermal well construction. BNL 51224, Vol. 1 and 2, December 1979.

6. T. SUGAMA, L. E. KUKACKA, and W. HORN. *J. Materials Science* **15**, 1498-1508, (1980).

7. J. J. FONTANA and J. BARTHOLOMEW. The use of concrete polymer materials in the transportation industry, BNL 28326. Proceedings of the American Concrete Institution Symposium Polymers In Concrete, San Juan, Sept. 24-25, 1980, (in press).

8. T. SUGAMA, L. E. KUKACKA, and W. HORN. Hydrothermal durability of Ca-polyester complexed polymer concrete, BNL 28092. *Cement and Concrete Research* (in press).

Environmental Sciences

INTRODUCTION

Programs relating to the environment and the impact of energy related activities are organized in four areas; Atmospheric Sciences, Environmental Chemistry, Oceanographic Sciences, and Land and Fresh Water Environmental Sciences.

ATMOSPHERIC SCIENCES DIVISION

The Atmospheric Sciences research program is designed to provide an improved understanding of the effects of energy production and use on air and precipitation quality. The program includes measurements and analyses of those meteorological factors which determine transport and diffusion of pollutants in the atmosphere, direct measurements of the vertical and horizontal distribution of atmospheric gases and particulates, measurements of contaminants in precipitation, tracer studies of transport and diffusion and modeling studies which deal with transport, diffusion, chemical transformations, and removal of atmospheric pollutants.

A major portion of the Division's effort is directed to the Multistate Power Production Pollution/Regional Acidity of Industrial Emissions project (MAP3S/RAINE) conducted in cooperation with other national laboratories. The emphasis of this project shifted in 1980 from a study of the regional scale transport of pollutants, primarily sulfates, to a study of wet and dry removal processes by which pollutants are removed from the atmosphere. Another major program is a continuing study of coastal meteorology and diffusion.

Research under the MAP3S/RAINE project includes modeling efforts aimed at improving the capability of predicting the atmospheric effects of emissions from fossil-fueled power plants. In support of this effort, measurements have been made to characterize existing air quality in the Northeastern United States and to investigate atmospheric processes that are important in the regional-scale transport and transformation of air pollutants.

The characterization measurements emphasize pollutant concentrations above the surface and are made from aircraft. Pollutants routinely measured are SO_2, SO_4, NO, NO_2, and light-scattering particulates. Meteorological measurements include temperature, relative humidity, solar radiation, and turbulence. Wind speed and direction are calculated from navigational measurements. The characterization experiments have been done in conjunction with intensive ground-based measurements conducted in the SURE program sponsored by EPRI. Current efforts are focused upon data interpretation and analysis.

Process-oriented experiments have been aimed at mechanisms leading to long-range transport. These have examined processes that mix pollutants to higher altitudes by making vertical profile measurements under various meteorological regimes.

Under the RAINE phase of the project, Division personnel are developing and adapting instrumentation for measuring cloud droplet characteristics and collecting cloud and rain drops from an aircraft for chemical analysis. These devices will be used with currently available meteorological and air chemistry instruments to investigate the processes by which pollutants are incorporated into clouds and rain. Analyses of hourly precipitation samples taken in all events since 1976 have shown significant relationships between meteorological conditions and air quality.[1,2] Recent studies are attempting to determine major source regions of the contaminants causing acidic precipitation. One such study involves calculation of air trajectories backward in time from the sampling site during precipitation periods. Concentrations are higher when the air has passed over a major industrial region such as the Ohio River Valley (Fig. 3).

References

1. G. S. RAYNOR and J. V. HAYES, Acidity and conductivity of precipitation in central Long Island, New York in relation to meteorological variables. *Water, Air, and Soil Pollution,* in press (1981).

2. G. S. RAYNOR and J. V. HAYES, Variation of chemical wet deposition by meteorological conditions. *Atmos. Environ.*, in press (1981).

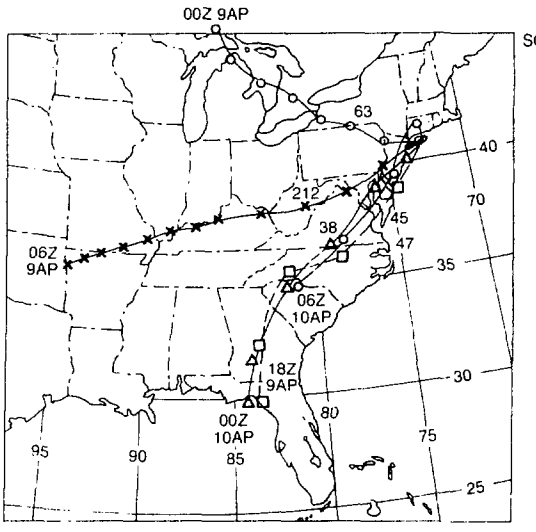

Figure 3. Air trajectories ending at BNL during a precipitation event. The sulfate concentration in the precipitation during each six-hour sampling period is shown beside the trajectory ending during that period.

ENVIRONMENTAL CHEMISTRY DIVISION

Research is directed toward the development and implementation of techniques to determine the concentrations of environmental pollutants arising from energy production and to study the interactions among them. Emphasis within the Division has been placed on developing highly sensitive techniques for measuring gaseous pollutants, developing methods for determining the size distribution and molecular composition of ambient aerosols, theoretical studies and laboratory measurements of aerosol properties, modeling the chemical reactions of pollutants, laboratory studies of the mechanisms and rates of fundamental reactions, field experiments to determine transformation mechanisms and rates of reactions occurring under ambient conditions, and field experiments to elucidate the interdependence of transport and transformation.

Theoretical Studies: 1) In a study of size effects upon the collision rates of aerosols it was identified that there is a weakening of the particle interaction potential energy due to retardation as particles increase in size.[1] 2) In application of the aerosol growth theory to a practical problem, namely, the light scattering properties of the well-known Los Angeles aerosol, it was shown for the first time that the extinction of light due to the presence of aerosol in the atmosphere depends on whether the aerosol components are present as homogeneous solution droplets of uniform concentration (internally mixed).[2] 3) In examination of removal of gaseous nitric acid by in-cloud and below-cloud scrubbing processes, the characteristic time for scrubbing of nitric acid by a cumulus cloud is the order of 5 sec and the characteristic time of rain-scrubbing was found to be of the order of 30 min, but depends strongly upon the assumed drop size distribution. 4) From 30 to 50% of the heat loss in buildings has been ascribed to air infiltration, the escape of heated air from a structure with replacement by cold, ambient air. A model for heat loss in buildings showed that by making periodic measurements of a tracer gas intentionally released at a controlled, known rate into each room of a building, the change in infiltration rate as a function of building construction and meteorological parameters could be determined.

Measurement Methodology: 1) Several photothermal dual laser schemes to perform *in situ* infrared absorption measurements of trace gases and aerosols were developed. Light from a tunable infrared laser absorbed by the species of interest induces photothermal changes which are subsequently probed using a visible laser.[3] 2) A Brookhaven-conceived atmospheric tracer sampler was designed to automatically sample the air for intentionally released perfluorocarbon tracers. These sampling and analysis tools now allow long-range (up to 1000 km) and complex terrain atmospheric dispersion and transport models to be adequately evaluated.

Laboratory Investigations: The stoichiometry of nitrogen oxide reaction with liquid water was determined by analysis of dissolved products to be $2NO_{2(g)} \rightarrow 2H^+ + NO_2^- + NO_3^-$.[4]

Field Studies: 1) The three and one half year plume study program at the Long Island Lighting Company (LILCO) oil-fired Northport Power Plant, comprising more than 60 airborne experiments, was completed and is probably the most extensive body of plume data ever gath-

ered from a single power plant. The typical rate of formation of sulfate in the plume indicates an apparent oxidation rate of less than 1% per hour. Diurnal influence or effects due to changes in various meteorological conditions were difficult to discern.[5] 2) Formation rates of sulfate and nitrate in the TVA Cumberland Steam Plant plume were determined and were tracked to distances of 200 km and 9 hours duration, where sulfate rate of formation varied from 0.1—0.8% per hour during night and early morning hours, and during late morning and afternoon ranged from 1—4% per hour. Rate of formation of nitrate exceeded the sulfate formation rates by a factor ~ 3.[6] 3) Atmospheric aerosol phase equilibrium experiments were carried out using techniques for real-time or short-interval determination of gaseous sulfur dioxide, ammonia, and nitric acid, and aerosol sulfur (sulfate), nitrate, ammonium, and strong acid.[7] The results indicate that ground level concentrations of ammonia are usually higher and nitric acid usually lower than predicted by phase equilibria calculations based on the aerosol composition.

References

1. W. H. MARLOW. Derivation of aerosol collision rates for singular attractive contact potentials. *J. Chem. Phys.* **73,** 6284 (1980).

2. I. N. TANG, W. T. WONG, and H. R. MUNKELWITZ. The relative importance of atmospheric sulfates and nitrates in visibility reduction. Presented at the Symposium on Plumes and Visibility: Measurements and Model Components, Grand Canyon, AZ, Nov. 10-14, 1980. *Atmos. Environ.* (In press).

3. A. J. CAMPILLO, C. J. DODGE, and H. B. LIN. Laser heterodyne interferometric detection of trace gases and aerosols. *J. Opt. Soc. Amer.* **70,** 1386-87 (1980).

4. Y. N. LEE and S. E. SCHWARTZ. Reaction kinetics of nitrogen dioxide with liquid water at low partial pressure. *J. Phys. Chem.* (In press).

5. J. FORREST, R. W. GARBER, and L. NEWMAN. Conversion rates in power plant plumes based on filter pack data, Part I: The coal-fired Cumberland plume. Presented at the Symposium on Plumes and Visibility: Measurements and Model Components. Grand Canyon, AZ, Nov. 10-14, 1980, *Atmos. Environ.* (In press).

6. R. W. GARBER, J. FORREST, and L. NEWMAN. Conversion rates in power plant plumes based on filter pack data, Part II: The oil-fired Northport Plume. Presented at the Symposium on Plumes and Visibility: Measurements and Model Components, Grand Canyon, AZ, Nov. 10-14, 1980, (Accepted).

7. R. L. TANNER. An ambient experimental study of phase equilibria in the atmospheric system: Aerosol H^+, NH_4, SO_4^{2-}, NO_3 — $NH_{3(g)}$, $HNO_{3(g)}$. Presented at the 180th National Meeting of the American Chemical Society, San Francisco, CA, Aug. 24-29, 1980.

OCEANOGRAPHIC SCIENCES DIVISION

The increasing utilization of coastal zones for energy-related activities has resulted in the location of about 200 fossil fuel power plants, 20 nuclear plants in operation or under construction, 12 major oil refineries, and 4 liquid natural gas terminals in the coastal zone of the northeastern U.S. (Fig. 4). The impact of these energy-related activities on the coastal marine ecosystem requires a careful evaluation of the processes and relationships between the physical environment and the biological components of the ecosystem. The BNL Oceanographic Sciences Division has continued the study of coastal marine ecosystems with emphasis on

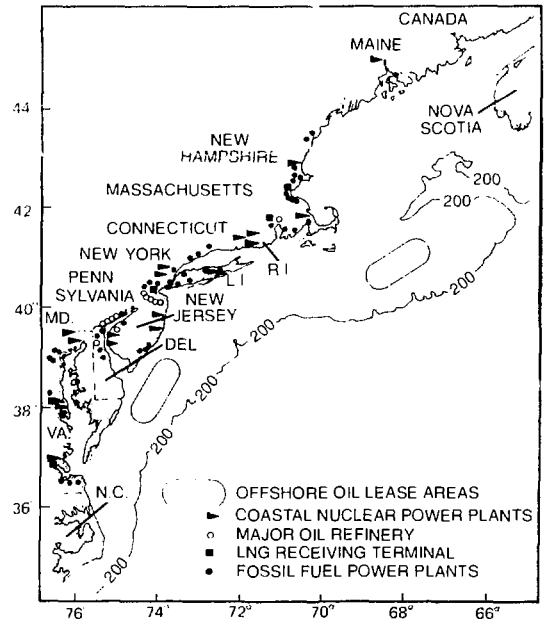

Fig. 4. Location of energy-related activities in the coastal zone of the northeastern U.S.

the coastal region from Georges Bank to Cape Hatteras in response to these needs.

From the analysis of large data sets collected during the last few years on numerous oceanographic cruises, and by moored instruments with line-of-sight and satellite telemetry, we have been able to describe the patterns of coastal water circulation and the seasonal changes in production and utilization of organic matter by pelagic and benthic communities. The average flow is from Georges Bank to Cape Hatteras along the continental shelf, with a mean velocity of 3 cm sec^{-1} and a transit time on the order of one year. Winter northeasterly storms contribute significantly to the westward water flow by increasing the velocity to ~ 10 cm sec^{-1}. The Nantucket Shoals/Georges Bank region is strongly influenced by tidal currents which produce intense vertical mixing of the water column. The southwestern part of the shelf is subject to freshwater runoff from estuarine discharge.

Studies of seasonal patterns of production and utilization of phytoplankton in the New York Bight and Georges Bank show that, contrary to earlier conclusions, as much as 50% of the primary production over the continental shelf is not consumed by zooplankton or respired in the water column and may be exported to the upper continental slope. From winter to early summer, consumption of phytoplankton by zooplankton accounts for less than 30% of the primary production. Only during late summer and fall is grazing pressure by zooplankton sufficiently great to control phytoplankton production.[1,2] A compilation of data on organic carbon and nitrogen in coastal and deep-sea sediments of the world's oceans[3] suggests that a large fraction of organic matter produced by phytoplankton may be accumulating in sediments of the continental slope. Furthermore, given the increase in primary production resulting from anthropogenic nitrogen inputs to coastal environments, this export could be a significant component of the total CO_2 budget and may account for the missing CO_2 emitted from burning of fossil fuels, but not observed in the atmosphere or mixed in the deep sea over the last 20 years.[4]

To evaluate the impact of energy-related perturbations on the coastal environment, it is essential first to understand the natural variability of ecosystems and the impact of natural perturbations. Extensive analyses of historical data and recent oceanographic and meteorological observations suggest that the anoxia observed along the New Jersey coast in the summer of 1976, which produced a $60 million loss to the shellfish fisheries, was the result of a casual chain of natural events. A warm winter with large runoff, low frequency of spring storms, and persistent southerly winds contributed to the formation of a deep summer thermocline, which, coupled with a low zooplankton grazing pressure, led to an anomalously large increase in the population of a dinoflagellate, *Ceratium tripos*, under the Hudson River Plume. The oxygen demand of these organisms exceeded the rate of surface resupply of oxygen to the lower part of the water column, resulting in anoxia.[5] On another front, the analysis of the impact of anthropogenic (overfishing) and natural (El Niño) perturbations of the Peru upwelling ecosystem suggests that the decline in anchovy biomass has led to apparent changes in the trophic-dynamics of the pelagic food web and in the properties of the water column. Following the steady decline in anchovy biomass since 1973, there has been an increase in the stocks of phytoplankton, zooplankton, sardine, and hake. As a consequence, the organic carbon content and sulphide production in the benthos has increased while dissolved oxygen in the water column has decreased. These changes in the coastal environment have also led to increases in the export of detrital carbon from this ecosystem.[6]

Because of the potential importance of phytoplankton production to problems ranging from coastal eutrophication to the global CO_2 budget, a symposium dedicated to the understanding of primary productivity in the world's oceans was held at BNL. Leading marine scientists in the fields of experimental biology and field ecology gathered to discuss marine primary production in relation to algal physiology and hydrodynamics.[7]

References

1. M. B. CHERVIN, T. C. MALONE and J. STEPIEN. Interactions between suspended organic matter and copepod grazing in the plume of the Hudson River. *Estuarine Coast. Mar. Sci.* (in press).

2. M. J. DAGG and D. W. GRILL. Natural feeding rates of *Centropages typicus* females in the New York Bight. *Limnol. Oceanogr.* **25,** 597-609 (1980).

3. E. T. PREMUZIC. Organic carbon and nitrogen in the surface sediments of the world oceans and seas: distribution and relation to bottom topography. BNL 51084, 118 pp. (1980).

4. J. J. WALSH, G. T. ROWE, R. L. IVERSON and C. P. MCROY. Biological export of shelf carbon: a neglected sink of the global CO_2 cycle. *Nature* (in press).

5. P. G. FALKOWSKI, T. S. HOPKINS and J. J. WALSH. An analysis of factors affecting oxygen depletion in the New York Bight. *J. Mar. Res.* **38**, 479-506 (1980).

6. J. J. WALSH. A carbon budget for overfishing off Peru. *Nature* (in press).

7. P. G. FALKOWSKI (ed.). "Primary productivity in the sea." In *Environmental Science Research*, Vol. 19, Plenum Press (1980).

LAND AND FRESHWATER ENVIRONMENTAL SCIENCES GROUP

The objectives of the current projects are to evaluate the effects of energy-related pollutants on selected species of forest and field crop plants, on soil microbiota, and on biota and biological processes in the freshwater ecosystem; to provide an ecological characterization of the BNL site and other sites preliminary to the possible establishment of a National Environmental Research Park; and a study of the relationship of environmental variables to virus survival and accumulation in aquatic organisms.

Effects of Acid Rain on Crops.

A treatment-response function was determined for the relationship between the hydrogen ion concentration of simulated acid rain (x) and the seed yield (y) of soybeans grown using standard agronomic practices and it can be expressed by the equation $y = 21.06 - 1.01 \log x$. The reduced yield may be caused by spray treatments which coincided with a sensitive stage in the life cycle of the plants or the cumulative effect of all rainfalls applied. Previous greenhouse studies[1] suggest that a cumulative reduction in total leaf area with increasing precipitation acidity may be at least partially responsible. Protein content of seeds also decreased. When expressed as seed protein per plant, plants exposed to pH 4.0, 3.1, 2.7, and 2.3 treatments exhibited reductions in protein content of 10.0, 19.2, 22.6, and 18.9%, respectively, compared to plants exposed to ambient conditions only. A one-percent reduction in yields of soybeans grown in the northeastern United States in 1979 would have resulted in a loss of 50 million dollars.

Effects of Acid Deposition on Forest Productivity

Acid precipitation is suspected of altering forest productivity. Changes could result from direct injury to live plants or indirectly through modification of soil properties and functions.

Simulation trials were carried out in two stages using two different models. The first stage used the forest growth simulator of Botkin *et al.* (JABOWA) modified to include the effects of nitrogen availability on tree growth. In these simulations, a pattern of nitrogen availability predicted following clear-cutting was reduced by 1/2, 1/4, and 1/10, and increased by 10 and 20 kg/ha/yr in five different trials. In the second stage, the feedbacks between production, litter fall, and future decomposition, and nitrogen availabilities are added by linking a much modified version of the forest growth model to litter production and decomposition models. This combined model is called FORTNIT (FOResT NITrogen model).

Our first set of simulations (JABOWA) indicate that even small changes in nitrogen availability due to acid rain will result in calculable short-term changes in production of these nitrogen-limited forests. However, when the further effects of altered productivity are included in the second set of simulations (FORTNIT), the results are complicated by temporal changes in the production/decomposition balance which determines net nitrogen mineralization. Clearly acid precipitation effects should be considered in this larger context but the accuracy of models on this scale is perhaps limited by a lack of knowledge of the types of materials classed as soil organic matter and their relative decomposition rates.

Effects of Lake Acidification on Biological Processes.

Acidification alters many aspects of lake ecosystems. Current work is centered on the hypothesis that materials cycling is reduced at low pH, leading to an accumulation of undecomposed litter and lowered nutrient availability. Work is conducted at Woods Lake (pH ~

4.9), Sagamore (pH ~ 5.5), and Panther Lake (pH ~ 7.0) in the Adirondack Mountains, a region heavily impacted by acid deposition. BNL efforts in the cooperative project are centered on the lakes, with studies of physical, chemical, and biological limnology in progress.

Analysis of leaf litter samples incubated for 220 days indicates that decomposition of beech leaves is inhibited in Woods Lake compared to less acidic Sagamore and Panther lakes. Of the five leaf species tested, red maple decomposed the fastest and red spruce the slowest in the three lakes.

Studies of benthic communities in these lakes support the hypotheses that acidification reduces the primary production and biomass of benthic microalgae and reduces the decomposition of organic material on the bottom. Statistically lower values of production and chlorophyll *a* were observed in Woods Lake, compared to the two less acidic lakes. Also the benthic decomposition is reduced under acidic conditions.

Aquifer Entrainment of Human Viruses.

A one-year project was initiated to assess the lateral movement of human enteroviruses through a shallow groundwater aquifer on Long Island. The study, funded by the Suffolk County Department of Environmental Health, has already identified the potential for viable virus movement through distances of up to 30 m from a subsurface septic source. Viral contamination of local drinking water has also been indicated by preliminary data.

Ecological Characterization of the BNL Site.

Populations of the white-footed mouse, *Peromyscus leucopus noveboracensis* (Fischer) were censused in xeric and mesic forests at BNL. Populations from xeric forests were small and ephemeral relative to those from mesic forests. Mouse distribution and abundance were dynamic and appeared to vary with habitat moisture and food resources levels. Significant seasonal trends in the somatic condition (body weight) of individuals remaining within habitats were observed. Movements by individuals between habitat types were also noted. These findings suggest that individual *P. leucopus* occupying the heterogeneous forest at BNL do experience changes in habitat quality and have the potential to respond to resource variation by selecting and exploiting local habitats opportunistically. Patterns of dispersal and habitat utilization are presently being investigated using radiotelemetry techniques.

Publications

J. D. ABER, G. R. HENDREY, D. B. BOTKIN, A. J. FRANCIS and J. M. MELILLO. Simulation of acid precipitation effects on soil nitrogen and productivity in forest ecosystems. BNL 28658, November 1980.

L. S. EVANS. "Foliar responses that may determine plant injury by simulated acid rain." In *Polluted Rain*, T. Y. TORIBARA, M. W. MILLER, and P. E. MORROW, Editors, pp. 239-257, Plenum Press, New York, (1980). BNL 27421.

G. R. HENDREY, N. D. YAN and K. BAUMGARTNER. Responses of freshwater plants and invertebrates to acidification. Presented at EPA/OECD Internat. Symp. for Inland Waters and Lake Restoration, Portland, ME, September 8-12, 1980. BNL 28534.

J. M. VAUGHN, E. F. LANDRY, C. A. BECKWITH, and M. Z. THOMAS. Virus removal during groundwater recharge: effects of infiltration rate on the adsorption of poliovirus to soil. *Appl. Environ. Microbiol.* (in press). BNL 28075.

Energy Technology

The Energy Technology Programs are directed to the development of advanced energy systems and components. Emphasis is placed on technologies that offer significant improvements in energy conversion and storage systems, the utilization of abundant and renewable sources, and significant improvements in environmental characteristics. Concepts that advance the state of the art beyond that required by current or contemplated standards are of primary interest.

OIL REFIT PROGRAM

In the area of fuel conservation the BNL Oil Refit Options Qualification Program has identified and quantified, by statistical sampling, the oil saving from a variety of refit options. These were systems operated in residential buildings where equipment was installed by a commercial firm at the direction of BNL. Options which qualified are now being marketed by firms in the industry. As a result of the program, a large body of data is now available at BNL on the performance of refit and newly available equipment, as well as oil use patterns in the northeastern U.S.

HYDROGEN STORAGE TECHNOLOGY AND HEAT PUMP SYSTEMS

The Chemical/Hydrogen Energy Systems Program in the Energy Storage and Conversion Division is a major effort and has an applications focus. The Hydrogen Technology Advanced Component Test System (HYTACTS) facility was made operational and used for conducting performance tests on a 22.7 kg capacity metal hydride hydrogen storage vessel. The Hydrogen from Small Hydropower project with New York State ERDA and the Village of Potsdam progressed through early study phases and submittal of federal environmental licensing documentation.

ELECTROCHEMICAL TECHNOLOGY

The oxidation of formic acid on single crystal Pt has been shown to be highly dependent on the crystallographic orientation.

Work on fuel cell systems has determined that the kinetic behavior of O_2 reduction on supported Pt and planar Pt are equivalent. It was also shown that oxygen reduction in 85% H_3PO_4 is enhanced by the addition of "catalytic" quantities of trifluoromethanesulfonic acid.

Systematic studies of the effect of additives on zinc electrodes has led to the development of a high rate insoluble zinc electrode with promising cycle life and shown the benefits of superimposed ac current during charging. This improvement increases the applicability of zinc electrodes in battery applications.

FOSSIL ENERGY TECHNOLOGY

Three new projects were started this year including one to develop a probe for the measurement of the mass of particulate matter in gas streams from fluidized bed coal combustors or gasifiers, a second dealing with the application of coal-oil mixtures to boilers in the commercial sector and a project to provide technical support to the Energy Regulatory Administration. These add to current fossil activities in catalysis, coal slurry combustion, hot combustion gas cleanup, gasification, system analysis, and fuel cell development.

Catalysis

A highly active series of Fischer-Tropsch catalysts, yielding hydrocarbons suitable for use as diesel and jet fuels, was developed. The method of catalyst formulation appears to be unique in the field of catalytic chemistry. These catalysts offer the promise of being superior to ordinary Fischer-Tropsch catalysts with regard to rate, operating conditions, handling techniques, longevity, and product selectivity. The "oxide mechanism" proposed to understand synthesis gas reactions was instrumental in guiding this development.[1]

These catalysts, in a slurry phase at 225°C and 8.3 MPa pressure, are 2000 times more active than those reported by the Bureau of Mines using conventional Fischer-Tropsch catalysts in fixed bed reactors. When compared with conventional catalysts in slurry reaction conditions, the new catalysts are 25 times more

active showing both the effectiveness and the usefulness of the slurry phase for hydrocarbon synthesis. Good selectivity for production of linear aliphatic hydrocarbons is observed over a range of temperatures and pressures.

Sulfur Removal from Hot Gases

Two approaches to sulfur removal from hot combustion gases are being investigated. Materials capable of being regenerated economically are a promising development, and a rotating fluidized bed absorber has been shown to be effective in removing SO_2 from hot combustion gases.

The sorbent, a calcium silicate class of cement, pelletized using a low cost agglomeration technique, was shown to be up to 15% more economical than current limestone sorbents now used in fluidized bed coal combustors. Laboratory tests proved they were resistant to attrition and capable of withstanding cycling through the sorption and regeneration stages of the process which can operate at temperatures up to 1000°C.

The rotating fluidized bed, using limestone sorbent, demonstrated better than 95% removal from gases at 850°C. Gas residence times in the bed were almost a factor ten lower than those necessary in conventional fluidized bed systems. A conceptual design study by an engineering firm further indicated the feasibility of this approach.[2]

Coal Combustion

A study indicated the feasilibility of using coal-oil-mixture (COM) fuels for boilers in the commercial sector where up to now the use of coal seemed to be unreasonable. A program leading to the demonstration of this application has been started.

References

1. W. SLEGEIR, R. SAPIENZA, and B. EASTERLING. "Mechanistic aspects of the homogeneous water gas shift reaction." *Catalytic Activation of Carbon Monoxide*, Peter C. Ford, Editor, American Chemical Society, Washington, D.C. 1981 (in press).

2. C. H. WAIDE, and H. SERRY. Feasibility of utilizing a rotating fluidized bed for the removal of sulfur from hot gases. April 1980, BNL 51253.

The Brookhaven House combines traditional home design with significant energy saving features.

SOLAR ENERGY TECHNOLOGY

The most visible accomplishments of the Solar Technology Program at Brookhaven National Laboratory (BNL) were: (1) the development of the low cost thin-film collector; completed modules could be sent to an independent laboratory for testing, and (2) the development of the ground-coupled heat pump technology; a residential system can be designed and sized with confidence and installed in a house on the BNL site. Performance results from the plastic film collector were better than those of the average comparable all-metal collector.

ENERGY CONSERVING ARCHITECTURE

The house designed under BNL's program in energy conserving architecture was built at the Lab site and instrumented to verify its thermal performance. The house is designed for passive solar heating, utilizing thermal storage in masonry walls covered by south-facing glass.

National Center for Analysis of Energy Systems

INTRODUCTION

The emphasis of the programs at the National Center for Analysis of Energy Systems is on energy policy and planning studies at the regional, national, and international levels. The Center carries out interdisciplinary studies of the technological, economic, social, and environmental aspects of energy systems. It is organized into four Divisions: Regional Energy Studies, Economic and Systems Analysis, Biomedical and Environmental Assessment, and Technology and Data. Development of planning frameworks, analytical models, data bases, and assessment provides the foundation for the energy studies. The program involves both operational support to DOE and original research in energy systems analysis.

REGIONAL ENERGY STUDIES DIVISION

Regional Assessments

During 1980, regional energy and environmental assessments were completed for the three federal regions in the northeast, in conjunction with other national laboratories and DOE's Divisions of Regional and Technology Assessment.[1-3] Such issues as water quality, socioeconomic impacts, solid waste impacts, coastal zone management, and long range transport of air pollution were considered.[4-12]

BESS (Brookhaven Energy System Simulator), a computer model dealing with the matrix algebraic representation and computation of reference energy systems was designed and implemented. This model accounts for refined oil product differentiation, and distinguishes between existing capital stock and that which must be added to meet some scenario requirement. It will be applied to ongoing regional assessments in the northeast.

A project to study the impact of government regulation on several selected industries, including the pulp and paper and the iron and steel industries, was started for the Technology Assessment Division.[13] Other industries will be considered during 1981.

Studies for the Nuclear Regulatory Commission

The Regional Energy Studies Division completed a large Siting Methods project for the NRC and several reports of that work are being published.[14-18] This project established guidelines for decision makers to follow when selecting sites for nuclear energy facilities. A summary document was completed for the NRC which set criteria by which the NRC can judge requests from DOE for future high level waste repository sites. It is anticipated that this project will continue next year with the emphasis on the legal and environmental aspects of high level waste siting as well as public involvement in the siting process.

International Programs

MARKAL, Market Allocation model was developed at BNL and has been implemented successfully in 15 nations as part of the International Energy Agency Phase II work. MARKAL is a multiperiod time-phased linear programming model to describe national energy systems over a 45-year period.[19] These results have been recently published by IEA in Paris. IEA Phase III will begin shortly and will serve to reconcile the differences between the MARKAL model here at BNL and the one at Kernforschungsanlage-Jülich (KFA) Germany.[20,21]

BEEAM, the Brookhaven Energy/Economic Assessment Model, was developed this year. This computer model projects gross output by energy sector, i.e., oil or natural gas for industry, private sector, etc. This model is currently being applied to Portugal and South Korea.

With support from the Agency for International Development (AID), studies on food and energy systems for Senegal[22] and the Dominican Republic[23] were completed. The second AID-supported Energy Management Training Program, which trains energy planners from various developing countries worldwide, was

held in conjunction with the Institute for Energy Research at the State University of New York, Stony Brook, and plans are currently underway for a third.

References

1. J. BRAINARD and J. S. MUNSON, Regional Issue Identification and Assessment Program (RIIA): Environmental Impacts and Issues of the EIA Mid-Mid Scenario: Federal Region I, April 1979, BNL 51135.

2. J. BRAINARD and J. S. MUNSON, Regional Issue Identification and Assessment Program (RIIA): Environmental Impacts and Issues of the EIA Mid-Mid Scenario: Federal Region II, May 1979, BNL 51136.

3. J. BRAINARD and F. W. LIPFERT, Regional Issue Identification and Assessment Program (RIIA): Environmental Impacts and Issues of the EIA Mid-Mid Scenario: Federal Region III, May 1979, BNL 51137.

4. E. KAPLAN, H. C. THODE, JR., and A. PROTAS, Relationships Between Rocks, Soils and Water Quality in the New England and Mid-Atlantic U.S.: Implications for Effects of Acid Precipitation on Surface Water, BNL 27261, January 1980.

5. E. KAPLAN and H. C. THODE, JR.; Water Quality, Energy and Socioeconomics: Path Analyses for Studies of Causality, *Water Resources Research*, (in press), BNL 28505.

6. P. M. MEIER, M. ROWE, R. MALONE, and G. KETCHAM, National Coal Utilization Assessment: A Systems Analysis of the Environmental Impacts of Increased Coal Utilization: Some Preliminary Results for the Northeast, BNL 51283, June 1980.

7. W. METZ, Socioeconomic Impacts of Proposed Power Plants in the Northeast: Issue Paper 1, BNL 51288, May 1979.

8. R. E. MEYERS, L. I. KLEINMAN, T-Y. LI, and R. T. CEDERWALL, Atmospheric Long Range Transport Lead Laboratory Methodology: Issue Paper 2, BNL 51289, Feb. 1981.

9. F. C. BRYANT, Selected Institutional Aspects of Energy Development in the Northeast: Issue Paper 3. BNL 51290, October 1979.

10. E. KAPLAN, A Methodology for Analyzing the Water Quality Impacts of Cooling Tower Blowdown: Issue Paper 4, BNL 51291, July 1979.

11. F. W. LIPFERT, A Methodology for Analyzing the Short-term Air Quality Impacts of New Power Plants: Issue Paper 5, BNL 5192, July 1979.

12. W. C. METZ, The Mitigation of Socioeconomic Impact in the Electric Utility Industry, *Power Utilities Fortnightly 106*, No. 6, 34-42 (1980), BNL-NUREG 27974.

13. W. ROGERS, S. BROWN, R. SHYPAILO, and P. M. MEIER, The Impact of the National Energy Plan on the Pulp and Paper Industry: An energy-environmental assessment, BNL 51311, October 1980.

14. B. PIERCE and M. ROWE, Quantitative Nuclear Power Plant Siting Methods: A Review of Current Practice, BNL-NUREG 28115, August 1979.

15. M. D. ROWE and B. L. PIERCE, A Comparison of Site Evaluation Methodologies, BNL-NUREG 51203, August 1979.

16. B. F. HOBBS, Analytical Multiobjective Decision Methods for Power Plant Siting: A Review of Theory and Applications, BNL-NUREG 51204, August 1979.

17. B. F. HOBBS and M. D. ROWE, A Comparison of Region Screening Methodologies, BNL-NUREG 51205, September 1979.

18. M. D. ROWE, B. F. HOBBS, B. L. PIERCE, and P. M. MEIER, Evaluation of Nuclear Power Plant Siting Methodologies, BNL-NUREG 51206, September 1979.

19. L. G. FISHBONE and H. ABILOCK, MARKAL, A Linear-programming Model for Energy Systems Analysis: Technical Description of the BNL Version, *International Journal of Energy Research* (in press).

20. D. HILL, V. L. SAILOR, and L. G. FISHBONE, Future U.S. Energy Technologies: Cost and Oil-import Trade-offs, *Science* (submitted), BNL 28798.

21. P. A. BERGENDAHL, Energy Systems Analysis for Sweden, 1980-2020: A Multiobjective Analysis of Options, Constraints, and the Contribution from New Technologies, February 1980.

22. Senegal Food and Energy Study: Energy Use and Opportunities for Energy-related Improvements in the Food System, Checchi and Company, Washington, D.C. in collaboration with Brookhaven National Laboratory, Upton, NY, August 1980.

23. G. MCGRANAHAN, G. MITCHELL, V. MUBAYI, and R. STERN, A Preliminary Assessment of Energy Supply and Consumption in the Dominican Republic, BNL 51202, November 1979.

ECONOMIC AND SYSTEMS ANALYSIS DIVISION

Integrated Energy and Economic Modeling and Analysis

An integrated technological and economic methodology has been developed for assessing the macroeconomic and energy system impacts of alternative energy policies.[1] This methodology takes into account the full range of complex interactions between the nation's energy and economic systems. The component models of this system include:

1. The Dale Jorgenson Associates; Dynamic Generalized Equilibrium Model (DGEM), a flexible interindustry representation of sectoral production and final demand. DGEM captures the combined influences of productivity, investment, and labor supply on the expansion of U.S. productive capacity over the long run;[2]
2. The Brookhaven National Laboratory and University of Illinois Input-Output model, a detailed interindustry model. This model calculates detailed estimates of labor, capital, materials, and functional end-use energy requirements given the aggregate demand and production information from DGEM *and* represents the interfuel substitutions obtained from the model below;[3] and
3. A detailed technological model of energy supply, conversion, and end-use demand, the Time-stepped Energy System Optimization Model (TESOM).[4]

A recent analysis performed with this system examined three possible energy strategies to access the economic, environmental, and national security benefits and costs of each policy. In the first strategy, no additional programs or policies are initiated beyond those in effect or announced in mid-1979. The second is directed toward reducing the growth in energy demand, i.e., energy conservation. The third promotes increased domestic supply through accelerated development of synthetic and unconventional fuels. The results indicate that conservation can substantially reduce import dependence and slow the growth of energy demand, with only a small macroeconomic cost and with substantial environmental benefits; the synfuels policy reduces imports by a smaller amount, does not reduce the growth in energy demand, involves substantial environmental costs, and slows the rate of economic growth. These relationships could be different if the energy savings per unit cost for conservation are less than anticipated, or if the costs of synthetic fuels can be significantly lowered. Given these uncertainties, both conservation and RD&D support for synfuels should be included in future energy policy. However, between these policy alternatives, conservation appears to be the preferred strategy.[5]

Solar Energy and Electric Utilities

The appropriate rates to be charged consumers who install solar space and hot water heating devices with electric utility back-up is a subject of continuing interest and controversy.[6] A companion issue is the matter of rates used in the exchange of electricity between consumers who own solar electric generating devices, who at times purchase and at other times sell electricity, and the utilities, with which they are interconnected. A model has been devised to measure the long run incremental cost incurred by utilities in providing back-up for solar heating devices which also measures the cost avoided by utilities in purchasing electricity from consumers who own solar generating equipment.[7] The model is also appropriate in estimating the economic impact on utilities of consumer-owned cogeneration.

Energy Consumption in Buildings and Community Systems

Activities in the area of energy consumption in buildings include development of analysis models, analysis of changing fuel and technology prices upon investment in energy conservation technologies and energy use, and development of data relevant to performing building energy use analyses.

The model development activities include the reformulation of Brookhaven Buildings Energy Conservation Optimization Model (BECOM) to better reflect new and retrofit technology options and explicitly include a wide range of tax, credit, and regulation policy parameters in the model. The new version of the BECOM model is also being implemented to allow analysis of community energy systems and their potentials for conserving energy in buildings. A second model development activity currently underway focused upon analysis of federal appliance

policies and their potential impacts upon purchases of durable goods by consumers.

Three major building energy analyses have been completed. The first was carried out in support of developing building energy performance standards at a federal level. This analysis considered building shell construction alternatives and identified relative economic efforts associated with different performance standard options. The second analysis explored a range of energy conservation policy alternatives under consideration by the New York State Energy Office,[8] and identified a set of policies that best met energy conservation goals and were not economically or institutionally unviable. The third analysis was carried out for the Mellon Institute and investigated the economics of using alternative air conditioning technologies under a range of assumptions on fuel prices and technological development in new devices.

The data development activities include general maintenance of existing data bases to keep them as current as possible. Also, new data necessary to support models under development have been assembled to allow testing of computer codes and validation of models themselves.

References

1. P. J. GRONCKI, and W. MARCUSE, The Brookhaven Energy Modeling System and Its Uses in Conservation Policy Analysis, BNL 51056, July 1979.

2. E. A. HUDSON, D. W. JORGENSON, and R. C. O'CONNOR, The Dynamic Generalized Equilibrium Model: Linear Logarithmic Specification, Report to Applied Economics Division, Federal Preparedness Agency, General Services Administration; Data Resources, Inc., August 24, 1978.

3. J. T. FRASER, Documentation of the Brookhaven Energy I-O and I-O/BESOM Linkage, BNL 50856, August 1978.

4. A. S. KYDES and J. RABINOWITZ, The Time-stepped Energy System Optimization Model (TESOM): Overview and Special Features, BNL 51095, August 1979.

5. H. DAVITIAN, R. J. GOETTLE, P. J. GRONCKI, E. A. HUDSON, P. KLEEMAN, and J. LUKACHINSKI, Strategic Cost-Benefit Analysis of Energy Policies: Overview, BNL 51105, October 1979.

6. R. BRIGHT and H. DAVITIAN, Electric Utilities and Residential Solar Systems, BNL 27711, April 1980.

7. R. BRIGHT and H. DAVITIAN, A Method for Computing Marginal Costs Associated with On-Site Energy Technologies, BNL 51264, August 1980.

8. P. T. KLEEMAN and D. SCHNEIDER, Analysis of New York State Energy Office Conservation Programs in Buildings, BNL 28523, September 1980.

BIOMEDICAL AND ENVIRONMENTAL ASSESSMENT DIVISION

The programs of the Biomedical and Environmental Assessment Division (BEAD) aim at providing scientifically-based, quantitative estimates of health and environmental risk and damage of energy supply and use. BEAD has a central, integrative role in DOE's Health and Environmental Risk Analysis Program. Results are used in planning and formulating energy technology and policy and in guiding energy related biomedical and environmental research. All energy sources are considered, although greatest attention has been given to coal, nuclear, photovoltaic, and conservation. Consideration is given to all phases of energy cycles — extraction, conversion, transportation, storage, and use — as well as to the effects throughout the economy of the materials needed to build and support the energy technology.[1-3]

An important emphasis in the Division is the development of new methods of health and environmental analysis and of new data bases, such as a listing of endangered species and critical habitat by county,[4] and a new environmental risk analysis method based on economic input-output analysis being developed in collaboration with the Economic and Systems Analysis Division.[5]

A large new program has been started in BEAD to assess health and environmental aspects of photovoltaic energy.[6-8]

BEAD analysis revealed that, while the Coal Mine Health and Safety Act has reduced the risk of fatal accidents to coal miners, almost all the gain has been offset by decreasing productivity so there has been very little decrease in accidental deaths per ton produced and nonfatal accident rates have increased.

BEAD analysis found no public health hazard associated with use of arsenic and cadmium in photovoltaic energy systems, contrary to previous reports in the literature.

References

1. L. D. HAMILTON. Comparison of health effects associated with various electric power generation systems: results and summary of work in progress in North America. Presented at the *European Scientific Seminar: Methods for Optimizing Protection in the Nuclear Industry,* Commission on the European Communities and Commissoria a l'Energia Atomique Euratom CEA Association, October 1979, (in press).

2. L. D. HAMILTON. Health effects of acid precipitation. *Proc. Action Seminar on Acid Precipitation, November 1-3, 1979,* A.S.A.P. Organizing Committee, pp. 117-134, Toronto, Canada, November 1979.

3. L. D. HAMILTON. Areas of uncertainty in estimation of health risks. *Proc. Symposium on Energy and Human Health, March 20-29,* EPA 600/9-80-030, pp. 513-17, Pittsburgh, PA May 1980.

4. J. NAGY and C. E. CALEF. ESUSA: U.S. endangered species distribution file. October 1979, BNL 51129.

5. M. D. ROWE and P. J. GRONCKI, Occupational Health and Safety Impacts of Renewable Energy Sources. September 1980, BNL 51307.

6. P. D. MOSKOWITZ, L. D. HAMILTON, S. C. MORRIS, K. M. NOVAK, and M. D. ROWE, Photovoltaic energy technologies: health and environmental effects document. September 1980, BNL 51284.

7. C. V. ROBINSON and K. M. NOVAK, Programs and subroutines for calculating cadmium body burdens based on a one-compartment model. August 1980, BNL 51306.

8. T. OWENS, L. UNGERS and T. BRIGGS, Estimates of occupational safety and health impacts resulting from large-scale production of major photovoltaic technologies. August 1980, BNL 51324.

TECHNOLOGY AND DATA DIVISION

The programs of the Technology and Data Division emphasize the technological characterization of all facets of the energy system[1,2] and the data associated with these technologies, which range from resource extraction, conversion, and transportation through final utilization in consuming sectors. Parameters and data of interest include capital and operating costs, process efficiencies, associated environmental emissions, and potential levels of implementation into the energy system. A basic tool used for analysis is the Reference Energy System, which is a network representation of all processes occurring in the energy system, and for which an appropriate set of coefficients is employed at each mode to characterize the technological processes of the system. Both existing and new technologies may be so characterized.

Programs in the Division are directed primarily toward the employment of new technologies and interfuel substitution in the energy system, and toward the potential implementation of such measures.[3-5] Included in the spectrum of such programs are the following:

- A district heating model[6-8] is under development to assess the potential penetration of this technology into the U.S. energy system.
- The impact of storage technologies associated with solar energy are under study[9,10] to estimate both economic tradeoffs and potential nonrenewable fuel savings.
- The potential penetration of advanced coal-combustion techniques into the electric utility sector is under investigation.[6,11-13]
- The development of a system for analyzing energy emergencies was completed, and the system is undergoing validation.[14-16]

References

1. M. BELLER, A consistent methodology for technology and policy impact assessment Presented at the workshop on Energy Policy Analysis, Urbino, Italy, October 1980. BNL 28412.

2. M. BELLER, Methodology for assessing the full costs of technology, *Energy Research* **4,** 235-251 (1980). BNL 26988.

3. J. LAMONTAGNE and L. RUFF, Synthetic fuels planning: a suggested approach. BNL 27315 February 1980.

4. E. A. CHERNIAVSKY, Long-range oil and gas forecasting methodologies: literature survey. BNL 51216 August 1980.

5. E. A. CHERNIAVSKY, Oil/gas supply modeling considerations in long-term forecasting. Presented at the Symposium on Oil and Gas Supply Models, Washington, DC, June 1980. BNL 28740.

6. P. GRONCKI, A. KYDES, J. LAMONTAGNE, W. MARCUSE, and G. VINJAMURI, Survey review of models for use in market penetration analysis (utility sector focus). BNL 51215 December 1980.

7. A. REISMAN and J. KARKHECK, Brookhaven National Laboratory district heating model: an overview. BNL 28251 October 1980.

8. A. REISMAN, A generic model for district heating: a geothermal application. Presented at the Workshop on Energy Policy Analysis, Urbino, Italy, November 3-7, 1980.

9. R. W. LEIGH, Storage in solar total energy systems. BNL 51230 December 1980.

10. R. W. LEIGH and R. W. POUDER, Fuel conservation potential of solar storage walls. BNL 51277 December 1980.

11. P. GRONCKI, H. HONG and J. LAMONTAGNE, Futures for electric power generation: three scenarios. BNL 27674 April 1980.

12. A. QUEIROLO, Survey of electric utility data sources with application to R&D planning. BNL 28242 August 1980.

13. J. LAMONTAGNE, P. LOVE and A. QUEIROLO, An approach to market penetration analysis for advanced electric power generation technologies. BNL 51285 December 1980.

14. A. HERMELEE, Correlation between energy use and indicators of energy consumption. BNL 28359 September 1980.

15. A. HERMELEE, J. D'ACIERNO, M. BELLER and T. A. SMITH, Situation report for petroleum exporting countries. BNL 51314 November 1980.

16. J. D'ACIERNO, Analysis of gasoline supply for the United States during the 1979 shortage. BNL 51330 December 1980.

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Department of Nuclear Energy

INTRODUCTION

The Department of Nuclear Energy (DNE) conducts programs that arise because of the possible use of nuclear properties as a source of useful energy. The program areas with which DNE is involved are advanced fission and fusion reactor systems; safety of fission reactors; compilation and evaluation of nuclear data; nuclear waste management; and nuclear materials safeguards, both domestic and international. Responsibility for research in these areas is assigned to various groups within the department. DNE is exceptional at BNL in that the bulk of its funding comes from the Nuclear Regulatory Commission (NRC) rather than from the Department of Energy (DOE). The present budget allocations are about 60% from NRC, 15% from DOE, and the remainder from other sources.

Nuclear Safety

Nuclear safety programs at BNL sponsored by the NRC consist of research to improve understanding of various types of reactors under hypothetical accident conditions, development of computer codes for accident analysis, risk assessment studies, waste management studies, and technical assistance to support day-to-day NRC reactor licensing requirements. Studies on three generic reactor types, light water, high temperature gas-cooled, and fast reactors, include both analytical and experimental work. Of course, the experimental work at BNL is not carried out with operating reactors.

CORE SAFETY AND PLANT TRANSIENT ANALYSIS

The core safety and plant transient analysis programs assist the NRC in establishing the capability of analyzing and understanding the behavior of a nuclear power plant during normal and abnormal operation. Calculations are provided NRC staff for their use in assessing the methods used by vendors and operators in calculating performance of their reactors, and the results of these calculations. This helps assure that the necessary degrees of accuracy and conservatism are present. In some cases, the main interest is in neutronic and thermal-hydraulic aspects of the core of the reactor; in others, more reactor components must be included. The areas of expertise used for these analyses include neutron transport, fluid mechanics, and heat transfer.

Studies have been done of possible rod drop accidents at a boiling water reactor (BWR). A control rod blade is assumed to have dropped out of the reactor; the reactivity addition would then cause a power surge which would be terminated by negative feedback due to an increase in fuel and moderator temperatures and the generation of steam voids. The effects of different reactor conditions and modeling assumptions have been studied. Some of the variables considered are initial power level, rod worth, speed of rod insertion, coolant flow rate, inlet subcooling, fraction of energy directly deposited in coolant and structures, and delayed neutron fraction. Emphasis was placed on the effect of feedback from expansion and boiling of the moderator, which is usually neglected. Based on these studies, it has been concluded that the reactivity feedback caused by void formation in BWRs provides a significant amount of conservatism during this accident.

Work is continuing to produce data sets for ready use in static and transient safety calculations at any point in a fuel cycle of a three-loop PWR and a BWR/3 design through Cycles 1 and 2. Cross sections for a four-loop PWR are being developed for use in a rod ejection accident analysis. Extensive comparisons have been made between calculations and observed perfor-

mance, which have been used to validate the calculational methods. The BNL system of core-follow codes was updated to make this process more efficient.

Work continues on topics pertinent to the radiation embrittlement of pressure vessels and shield tanks. The spectral lead factor which relates surveillance capsule measurements to pressure vessel fluence has been studied and procedures used by Industry have been improved. Fluences generated in the Pool Critical Assembly Pressure Vessel Dosimentry Experiment have been calculated, and these results will be considered as a benchmark. Specific one- and two-dimensional multigroup transport theory calculations of fluences and damage levels are being done upon request from NRC.

Some of the brief studies done to provide NRC with rapid technical assistance when needed are the following: (1) Monte Carlo criticality calculations were performed to assess safety of storage racks for reactor fuel; (2) calculations were made of effects of various reactivity perturbations which might explain power "tilts" at operating reactors; and (3) calculations were also done to relate the readings of power range instruments at operating plants to control rod patterns and core power level.

The plant transient analysis programs provide technical assistance to the NRC in the analysis of transients at both BWRs and PWRs. The programs include the modification of large computer codes to accommodate specific NRC requirements. The IRT computer code was purchased from a reactor vendor and was considerably modified to meet NRC needs. Documentation and preparation for release of the revised code is essentially complete. IRT is a fast running code for analysis of PWR systems. In its revised form, it will be used for transient calculations.

A large analytical program was completed on Anticipated Transient Without Scram (ATWS) for both boiling water and pressurized water reactors. This program, which was initiated following the Three Mile Island incident, includes the effects of a stuck open primary side relief valve during various transients where the scram system is assumed to be inoperable.

Following the recent incident at Brown's Ferry where the steam system was automatically shut down but only a fraction of the scram rods were inserted, DNE staff was requested to perform an analysis of this event. Of particular interest were the effect on the containment suppression pool temperature and the ability to shut down the reactor completely. Results of these analyses have been transmitted to NRC staff and have been used during various presentations to NRC.

A new analytical model of a once-through steam generator (OTSG) typical of a Babcock and Wilcox reactor was incorporated in the IRT code. This model was designed to improve the computational speed of calculations involving the OTSG, and has provided excellent agreement with previous calculations.

A new program was initiated to provide an analysis of the Departure from Nucleate Boiling Ratio (DNBR) in a sixteen fuel rod bundle test being performed at Columbia University.

REACTOR SAFETY EVALUATION

An evaluation was performed of the reduction in risk that would be achieved if equipment used to bring a pressurized water reactor to cold shutdown conditions were made safety grade. A limited risk analysis was performed for pertinent accident sequences, including earthquakes and loss of offsite power, and it was found that only for the earthquake initiator would there be a signficant reduction in the probability of a disabling accident (by approximately one order of magnitude) if safety-grade equipment were used.

As a pressurized water reactor is brought to cold shutdown under natural circulation conditions, adequate boration of the primary coolant must be assured in order to maintain subcriticality. Plans are currently underway for tests on nuclear reactors to ascertain whether adequate mixing of boron occurs during the natural circulation flow transient. In order to provide pretest guidance to the NRC, BNL has developed a computer model BITRAN (*B*oron *I*njection *TRAN*sient) of the primary coolant system which describes the boron injection and subsequent distribution during the natural circulation transient. Documentation of the first version (for Westinghouse-designed reactors) of the computer code has been completed and preliminary results of the code are being used to define measurement requirements for the planned tests.

A significant activity was undertaken this year on evaluation of accidents leading to a degraded core. The main thrust was analysis of severe hypothetical core meltdown accidents for the Zion and Indian Point Nuclear Plants. This work was performed in connection with an NRC question as to whether these plants could pose a disproportionate risk because they are in areas of high population density. In the studies, specific attention was given to accident sequences initiated by loss of offsite power and by small pipe breaks. Additional failures of engineered safety features were assumed for particular sequences. The thermal and physical transient response of the reactor vessel and the containment building were computed, with the MARCH code and BNL modifications of the code, for the following phenomena: core heatup, vessel depressurization, core slump, reactions between core debris and water, vessel failure, interaction between core debris and concrete, hydrogen combustion, and steam pressurization of containment. The effects of mitigating safety features were considered in connection with these transients. These include core retention devices, hydrogen control systems, and filtered, vented containment. Preliminary results were obtained for several accident sequences.

The owner of the Zion Nuclear Plant has conducted a residual risk study which identifies differences from the reference plant in WASH-1400. These differences in characteristics of the plants cause different calculated system reliabilities and risk perspectives from those calculated in WASH-1400. BNL has performed, at the request of NRC, a critique of the Zion risk study and an independent assessment of the dominant accident sequences which contribute to the risk. BNL estimates include a large probability of the Category 2 release defined in WASH-1400, as a result of an extended total loss of power coupled with failure of the turbine-driven pump train in the auxiliary feedwater system. Potential common mode failures in the engineered safety features were included in the BNL analysis and this led to a larger probability of core melt resulting from loss of coolant accidents.

The Office of Nuclear Reactor Regulation is developing a system interactions program to define and subsequently implement regulatory requirements and guidance as to systems interactions in light water reactor plants. Adverse system interactions would involve dependent faults among reactor systems which could lead to the loss or degradation of a safety function and to the potential for radiological consequences. BNL has reviewed and identified methods which could be developed as part of a procedure for finding and evaluating systems interactions. A preliminary procedure has been outlined and tested against specific reactor events that have occured.

CONTAINMENT SYSTEM INTEGRITY

The boiling water reactors (BWRs) designed by the General Electric Company (GE) incorporate large pools of water as part of the containment design. The purpose of the water is to serve as a large heat sink for condensing steam that could be released into the containment building during a loss of coolant accident (LOCA). This condensation would prevent excessive buildup of pressure inside the containment. To date, three different pool configurations have been used for BWRs; these are designated Marks I, II, and III. The BWRs currently operating in the U.S. are all of the Mark I type. The newer plants, now under construction, use Mark II and Mark III containment designs.

BNL's major role in connection with these containment designs is to assure that hydrodynamic loads that might be caused by a hypothetical LOCA or a safety or relief valve actuation are estimated in a technically sound and conservative manner. To perform this function, BNL staff advises NRC on the technical merits of the methods proposed by GE or the utilities for calculating such hydrodynamic loads on the pool walls and on structures located in and above the pools.

In work related to Mark I containments, BNL staff assisted NRC by providing information used in preparing the Mark I Safety Evaluation Report (NUREG-0661, July 1980). This document addresses, on a generic basis, all the containment-related hydrodynamic loads that could occur in Mark I plants. BNL personnel also served as NRC consultants when positions taken in this document were presented to the Advisory Committee on Reactor Safeguards (ACRS) on February 9, 1980. In work related to Mark II containments, BNL staff assisted NRC in preparing information used in Supplement

No. 1 to NUREG-0487 (August 1980). This document contains BNL's evaluation of new methods proposed by the utilities to estimate containment loads subsequent to publication of the original NUREG-0487. BNL has also continued to monitor progress on numerous test programs aimed at providing more accurate information on loads on Mark II containments. At NRC's request, BNL staff witnessed the full-scale Mark II condensation tests at the JAERI facilities in Japan (June and October 1980). In connection with the Mark III program, BNL has conducted in-depth review of GE's Interim Containment Loads Report. A formal set of NRC questions resulted from the review.

In addition to the hypothetical LOCA event, actuation of a safety relief valve (SRV) could also cause discharge of steam into the pool, with accompanying hydrodynamic loads. Unlike a LOCA, however, SRV actuation is a normal event that is expected to occur many times during the life of a reactor. BNL has reviewed numerous test programs (in the U.S. and abroad) aimed at providing a better evaluation of these loads. Of particular interest during 1980 has been the specification of a way to calculate loads that would be produced by simultaneous activation of several SRVs. BNL evaluations of SRV actuation load methodologies have been communicated to the NRC in numerous letter reports. Some of these have also been incorporated into the Mark I Safety Evaluation Report (SER) and Supplement 1 of Mark II SER.

FIRE PROTECTION AND DETECTION RESEARCH

This program includes studies on propagation, detection, and suppression of fires as related to nuclear safety. Models are being developed that will be used as a basis for NRC standards and NRC review of systems to mitigate the potential impacts of fires on the ability to shut down an operating reactor safely. This task includes study of fire plume growth, effects of fire suppressants on electrical equipment, and methods of optimizing the siting of early warning devices for fire detection.

STRUCTURAL ANALYSIS

The Structural Analysis programs provide assistance to the NRC and the DOE in the areas of seismic design and analysis, structural behavior, stress analysis, and structural reliability. The current programs include the following: Piping Benchmark Development, Confirmatory Piping Analysis, Review of Dynamic Qualification of Safety Related Electrical and Mechanical Equipment for Operating Licensed Plants, Pressure Boundary Fracture Toughness Requirements, and Development of Reliability Based Design Criteria for Nuclear Seismic Category I Structures.

In the Piping Benchmark program, benchmark problems for dynamic analysis, uniform support motion, and response spectrum methods were completed and results were published for the NRC. Currently, a set of piping benchmark problems for dynamic analysis, by the independent support motion response spectrum method is being developed. In the program on Review of Dynamic Qualifications of Safety Related Electrical and Mechanical Equipment, the Department is assisting the NRC's Equipment Qualification Branch in evaluating the dynamic tests by licensees for the seismic qualification of pumps, valves, and electrical equipment. In the program on Pressure Boundary Fracture Requirements, requirements for fracture toughness of components with complex shape are being developed. In the program on Reliability Based Criteria for Nuclear Seismic Category I Structures, the department is developing probabilistic methods for structural evaluation of nuclear structures in seismic category I.

LWR CODE DEVELOPMENT, ASSESSMENT, AND APPLICATION

RAMONA-3B is a code for calculating boiling water reactor transients. It was developed by Scandpower A/S and then purchased by BNL for the NRC. The advantage of this code is that not only does it model the steam supply system but it also models the core with three-dimensional neutronics.

In order to make the code into a production tool capable of use in calculating abnormal operational transients and hypothetical accidents of interest to the NRC, BNL has had to make many improvements. Models for the steam separators, jet pumps and drive pumps, and the steam line were added to the original code. A plant protection and control system was

added in order to allow for automatic scram, feedwater variation, drive pump trip, and activation of the different valves along the steamline. The fuel rod heat conduction model was improved and a new cross-section formalism was added to make the code compatible with other BNL core transient analysis codes. The code was assessed through comparisons with data from heated channel experiments done with 36-rod clusters, and from turbine trip tests at the Peach Bottom-II reactor.

A program was started in 1979 to provide NRC with independent assessment of various released versions of the TRAC code which were developed at Los Alamos Scientific Laboratory (LASL). Since last October, the scope of this program has been expanded to include application of the TRAC code to analyze various hypothetical accidents and plant transients, and assessment of the RELAP5 code which was developed at Idaho National Engineering Laboratory (INEL). The program also assists NRC in the assessment of the computations of various National and International Standard Problems.

The objective of the assessment task is to review the thermohydraulic models and correlations included in the codes and to simulate various separate effects tests to show the strengths and weaknesses of the code in predicting thermohydraulic phenomena which would be important under accident conditions. So far, many steady and transient one-dimensional tests and multidimensional tests have been modelled with TRAC-P1A and TRAC-PD2. Our experience with TRAC-PD2 indicates that there is still some room for improvement in the code, and NRC has been informed of this. After the RELAP5 code has been made operational on the BNL system, this code will also be used to simulate some separate effects tests.

This program will also apply a released version of the TRAC code to the analysis of various accidents and plant transients such as an overcooling transient or steam line break. The overcooling transient for the Rancho Seco Power Plant is currently being analyzed with TRAC-PD2. It has been found that the TRAC-PD2 neutronic model does not contain reactivity feedback, which could become important for some plant transients. Therefore, a reactivity feedback model is being incorporated into the TRAC-PD2 code to improve its capability.

SIMULATOR IMPROVEMENT

Two typical simulators currently used for the training and requalification of nuclear power plant operators have been reviewed for the Division of Reactor Safety Research. The assessment of thermohydraulic modeling assumptions has shown that simulators are currently limited to normal start-up, load-following and shut-down transients, and to minor deviations from normal operating conditions. Modeling improvements are required to extend the capabilities to accident conditions, as recommended by the President's Commission on the Accident at Three Mile Island.

To meet this requirement, the simulator improvement program is designed to establish the basis according to which existing training simulators can be supplemented by a special-purpose, high-speed peripheral processor and its specifically developed software. The new processor would simulate the thermohydraulic processes in the nuclear steam supply system, while the host computers presently in the simulators would continue to simulate the balance of the plant. The upgraded simulator could also be used to train operators to respond to hypothetical accident conditions, to carry out realistic engineering analyses at higher computing speeds than presently possible, to diagnose plant conditions during and after an accident and to select the optimum strategy for returning the plant from accident to safe shut-down conditions.

Manufacturers of simulators will cooperate with BNL to establish the link between existing simulators and the new processor.

RISK CRITERIA DEVELOPMENT AND HUMAN ERROR ANALYSIS

An assessment is being made of the practicality of utilizing risk criteria in the licensing of nuclear power stations. Implications of using quantitative risk criteria in this way will also be examined. Surveys are being performed to collect and analyze relative risks to society from a broad range of activities. Previously proposed risk criteria are being studied and related to results of the Reactor Safety Study and new developments in risk assessment since WASH-1400 was issued. Uncertainties in risk are also being incorporated in the criteria. The concepts

of total risk, core melt, and the consequences are being investigated as to their implications for risk criteria.

This program will lead to a formal process for evaluating the criteria which have been proposed, such as by the IEEE working group on risk criteria, the NRC staff, the ACRS, and the Atomic-Industrial Forum. A peer review group would be set up to critically review the criteria and their attributes. In addition, the project is developing a computer code using the PWR fault trees and event trees of WASH-1400, to permit recalculation with varying input data. This will permit use of human factors data developed by BNL last fiscal year.

The object of the Human Error Analysis work is to identify, classify, and rank the contributions to risk of human actions during the operation of nuclear power stations. In addition, the most effective means to increase safety through reduction of human error will be identified. Future analyses, design changes, and procedure changes necessary to realize the human error rate reductions will be identified elsewhere, and reviewed here.

In the FY 1980 task, Licensee Event Reports (LER) were analyzed to determine rates of valve misconfigurations and of failures of pumps to start, due to human error. During FY 1981, these error rates will be analyzed for patterns or anomalies related to specific plants, type of procedure, or other performance-shaping factors. The error rates will also be compared with those predicted by NUREG/CR-1278 and differences identified. In accomplishing this, BNL will, to the extent possible, develop sequences of actions involved in the above errors. The LERs will be sorted according to these more detailed sequences and respective human error rates calculated.

The program will use the same methods that were applied to pumps and valves in FY 1980 to develop estimates of human error rates for electrical equipment from LER data.

The last task in the program on analysis of human error rates is to prepare all necessary groundwork and develop agenda and an attendee list for a follow-up meeting to the Myrtle Beach Meeting (Proceedings of the Myrtle Beach Meeting on Human Factors and Nuclear Safety, December 2-7, 1979).

RELIABILITY MODELLING

In FY 1980, the FRANTIC code was modified to incorporate the Weibull failure distribution where the status after testing can be as good as old or as good as new. This program will develop a set of comprehensive sensitivity studies to demonstrate the implications of these alternatives on system unavailability.

In addition, BNL will develop the theory and software for FRANTIC, to be used to calculate failure occurrence rates and failure to operate for arbitrary time periods. The project will develop the theory and software to handle situations where a component in standby may have a different reliability behavior (e.g., exponential) from the behavior in operation (e.g., Weibull).

As part of this effort, BNL will develop a set of guidelines to be used in the licensing process that will consider scheduled as well as unscheduled downtimes in establishing limiting conditions for operations. The ratio method, where the maximum downtime is determined by allowing the accident probability during the interval to be no greater than some fraction of the baseline time period used, will be investigated. This program will develop bases for the baseline time period to be used for both unscheduled and scheduled downtimes. As failure distributions, the project will consider both exponential and Weibull distributions. BNL will also develop the theory to incorporate repair time distribution considerations into the ratio method. The program will modify the FRANTIC code so that allowed downtimes can be automatically computed from the ratio method.

THERMAL-HYDRAULIC SAFETY EXPERIMENTS FOR LWRs AND LMFBRs

The objective of this program is to develop and experimentally evaluate models of thermal-hydraulic phenomena relevant to reactor safety issues and in support of NRC code development programs. The experiments related to light water reactor safety address two aspects of reactor containment during postulated core meltdown accidents: core-concrete interactions leading to penetration of the basemat, and containment pressurization by thermal interaction between core debris and water.

The objective of the program on interaction between the core and the concrete is to develop

heat transfer models to describe the complicated interactions which contribute to the attack of molten core material upon the reactor cavity basemat. Experimental work is underway to simulate the phenomenon of interfacial heat transfer between superposed immiscible liquid layers composed of core oxides and metallic components which are being agitated and mixed by intense gas release from the lower surface. The heat transfer models developed will be incorporated into specific systems codes for calculation of the extent and rate of penetration of molten core materials into the concrete basemat.

Currently used containment codes predict that steam generated by interaction of molten core debris with cold water would lead to containment pressures which exceed the design limits of a containment building. An experiment has been designed to evaluate the models used in these codes. Simulated hot core debris will be dropped into cold water. The rate of steam generation will be measured, along with associated pressures and temperatures. The data will provide guidance for development of models to characterize the steam generation rate during the thermal interaction between the debris and the water.

The liquid metal fast breeder reactor (LMFBR) experiments include studies of phenomena related to aspects of the transition and post-accident heat removal phases of core disruptive accidents. An experimental simulation of the multiphase flow characteristics of boiling mixtures of uranium dioxide and steel has been carried out in support of analyses of the transition phase. Void fraction measurements were made in an adiabatic air-water bubbling column with gas injection. A traversing gamma densitometer was used to measure void fraction. The results of the study support earlier BNL conclusions from boiling studies that vapor generation during the transition phase can reduce the potential for fuel collapse and nuclear recriticality. It was found, however, that the gas flow in the gas injection experiments was less efficient than internal vapor generation from the standpoint of supporting the liquid in a dispersed configuration.

A study was completed of the feasibility of using microwave dielectric heating to simulate the nuclear heat source in transition phase boiling simulation experiments. The results indicate that heating of a boiling liquid in a microwave oven is likely to lead to non-uniformities in heat generation which cannot be predicted with state-of-the-art techniques. Furthermore, use of water to simulate sodium would further intensify the non-uniformities. A single-mode microwave waveguide concept was proposed which, together with a low index of refraction dielectric liquid, would provide a system with minimized heating non-uniformities.

An experimental and theoretical program on natural convection heat transfer in internally heated liquids was completed. Measurements of local heat transfer to vertical boundaries were made and correlated to appropriate modeling parameters. Theoretical boundary layer analysis was developed and solutions were compared to the data. In general, the analytical predictions were in agreement with the experimental data for local heat flux within ± 3%. Models developed from this program may be used for calculation of distributed heat loads under conditions where molten core material comes in contact with vertical structural barriers.

An experimental simulation of the freezing of multiphase fuel mixtures in LMFBR blanket regions was performed. Gas-liquid mixtures and solid-liquid slurries were used to represent the reactor materials. It was found that the presence of the dispersed phase in the flowing mixture accelerated the feezing process. However, the slurry freezing rate was measured to be as much as 100 times greater than the corresponding gas-liquid freezing rate. This study indicated that when a molten nuclear fuel mixture contains a dispersed second phase, the rate of freezing may be accelerated. In the case of a dispersed solid phase, the material may freeze so fast as to trap much of the fuel in the original core location and retard fuel dispersal.

Studies of the distributed boiling characteristics of internally heated liquids have continued. It has been found that prediction of the pool-averaged void fraction is in reasonable agreement with experiments. However, the local distribution of vapor as calculated is in poor agreement with available experimental data. The pools were observed to behave in a stratified fashion, with an intensely boiling region on top of a lower non-boiling region. Models have been developed to characterize this behavior, which predict the non-boiling depth as well as subsequent void distribution. These studies in-

dicate that although dispersive mechanisms exist in internally boiling liquids, significant non-boiling regions may exist which have previously been neglected in molten core safety analyses.

SYSTEM-WIDE REACTOR TRANSIENT CODE

The analytical simulation of a LMFBR system or a light water reactor (LWR) system for a variety of off-normal and accident conditions is an essential part of overall safety evaluation. Some of the examples of transient conditions of interest include the withdrawal of control rods; pump seizure in one of the heat transport loops, afterheat (decay heat) removal via natural circulation; and, for LMFBRs, a major pipe rupture in the sodium-carrying heat transport system. For any of these disturbances, the system response (i.e., temperatures, pressures, and flow rates at key locations) for the entire plant needs to be calculated to help the NRC in licensing studies.

To develop analytical tools for such applications, the Super System Code (SSC) Project at BNL is funded by the Division of Reactor Safety Research, NRC. This project has two elements, SSC Development and SSC Validation. Under the SSC Development program, work is progressing on four versions of the SSC series of codes. These are (1) SSC-L, which simulates the thermohydraulic response of the loop-type LMFBR; (2) SSC-P for pool-type LMFBRs; (3) SSC-W for water reactors; and (4) SSC-S for shutdown (i.e., long term) transients of the -L, -P and -W versions.

SSC is being developed as a highly generalized code. It has been designed to be user oriented, highly modular, and flexible. There is one central program library which contains all the subroutines for the various reactor system components/models, input processing, and output processing. How these computational blocks are interconnected internally in the code, and what input is used, distinguishes one version of SSC from another.

The SSC-L code has been operational since September, 1977. Reports describing not only the models and methods employed, but also detailed input requirements have been published. The code is presently available to all U.S. users directly through BNL. To date there are seven external users of SSC-L within the U.S. Foreign governments and parties can also obtain this code via agreements between them and the United States. Japan has acquired the code. The Federal Republic of Germany already obtained the code through bilateral agreements. Thus, SSC-L has moved from a purely developmental program into the area of applications.

The SSC-P code has been operational since November 1979. Documentation is now available[1] and the code is undergoing extensive testing before its official release. This code will provide an advanced analytical tool for accident analysis in any pool-type LMFBR. Examples of this type of reactor include EBR-II (the only operating fast breeder reactor in the United States), PHENIX and SUPERPHENIX in France, PFR in the United Kingdom, and others.

A major program milestone was reached in March, 1980, when the SSC-W code became operational at BNL. This version allows the more accurate prediction of natural circulation transients as well as other operational transients in LWRs while at the same time achieving computational speeds of better than real time simulation. Results of initial applications have already been reported.[2]

Work is continuing in several areas of SSC-S development. The development of models for several aspects important for long term transients is being conducted. These areas include adequate inclusion of intra- and inter-assembly effects; models for auxiliary/emergency cooling systems; and any additional required numerical techniques.

The SSC Validation program is designed to calibrate and qualify the SSC series of codes by applying them to actual test conditions and comparing predictions with results obtained from the test data. Emphasis is currently being placed on detailed analysis, using SSC-L, of preoperation and acceptance tests in the Fast Flux Test Facility (FFTF). A report detailing the pretest predictions utilizing SSC has been prepared.[3] In addition, studies have been completed to compare the results of SSC to those of similar, although analytically simpler, system codes (e.g., the DEMO code for the CRBRP and the IANUS code for the FFTF).

References

1. I. K. MADNI and E. G. COZZOLI, "An Advanced Thermohydraulic Simulation Code for Pool-Type LMFBRs (SSC-P Code)", BNL-NUREG-51280 (1980).

2. J. G. GUPPY, *et al.*, "Analysis of Natural Circulation Events in B&W Plants Using SSC-W", *Trans. Am. Nucl. Soc.*, **35**, 315 (1980).

3. L. G. EPEL, *et al.*, "Preliminary Pre-Test Analysis of FFTF Loss of Power Acceptance Tests", Brookhaven National Laboratory, BNL-NUREG-27116 (1980).

HIGH TEMPERATURE GAS COOLED REACTOR SAFETY EVALUATION

The High Temperature Gas-Cooled Reactor (HTGR) is a thermal reactor with a ceramic fuel (oxide or carbide) incorporated in a graphite moderator cooled by helium. The use of stable core materials permits exit coolant temperatures of the order of 800°C. The BNL program provides research support to the NRC in its evaluation of the safety of HTGR systems.

The long term effect of traces of impurities in the helium coolant on the graphite and metallic components of the reactor internals is being investigated to determine mechanisms of possible structural degradation. Experiments in recirculating He loops are helping to clarify the kinetics and equilibrium reactions taking place between the reactor internals and the trace impurities in the helium and to understand the mechanisms of transport of fission products through graphite at high temperatures.

ASSISTANCE TO NRC IN NUCLEAR WASTE MANAGEMENT

The Department continues to provide support to the NRC in the area of technical assistance and research for high level and low level nuclear waste. The effort addresses the long-term isolation of high level waste, transuranic wastes, and spent fuel.

In the low level area, BNL provides assistance on various problems related to shallow land burial. In the past year, experimental studies and technical assistance were begun on the disposal of waste generated from the cleanup of water in the auxiliary and containment buildings of TMI-2.

The experimental program in low level waste management included continuation of investigation of leaching of solid radioactive waste and waste containers, and the study of commercial low level radioactive waste disposal sites.

Property determinations were conducted on types of simulated waste forms currently produced at nuclear reactors. Data were developed to determine envelopes of process parameters within which there is reasonable assurance that satisfactory solidification will occur. These data will be compared to observations made on solidified reactor waste, and will provide the technical bases for establishing criteria for the safe disposal of solidified radioactive wastes.

Trench waters from the Maxey Flats, Kentucky, and Barnwell, South Carolina, disposal sites were sampled using an anaerobic collection procedure designed to preserve the *in situ* chemistry. The samples were analyzed for organic, inorganic, and radiochemical components. Water samples from experimental trenches constructed at Maxey Flats for the purposes of intercepting groundwater flow paths were also collected and analyzed. Trench water chemistry indicates that two processes, leaching of the wastes and bacterial degradation of organic matter discarded in the waste trenches, are occurring.

Sorption coefficient (K_d) studies using batch and column techniques are in progress. The purpose of these studies is to predict radionuclide movement and formulate guidelines for testing the retention capacity of potential disposal site geomedia. Gel-filtration chromatography experiments have been performed to detect the presence of organo-radionuclide associations in trench waters.

CORROSION SCIENCE

The Department has research programs in the Corrosion Science area with DOE and NRC, as well as technical assistance programs with two division of NRC. For the DOE Division of Basic Energy Sciences, the group has a continuing research program on mechanisms of intergranular stress corrosion cracking of iron- and nickel-base alloys. Work during the period concentrated on the intergranular stress corrosion cracking of stainless steels in low temperature water environments and the complex interactions between electrical potential, oxygen con-

centration, stress, and straining rates on the initiation and propagation of cracks. A major role of sulfur compounds, both present in solution and/or produced by the initial corrosion process, in accelerating the rate of crack propagation was discovered during this period. For the DOE Division of Geothermal Energy, the group has been monitoring the development of metallic materials for use in the geothermal industry, and has been performing in-house research on development of materials with improved pitting resistance to geothermal brines. A major discovery has been that additions of significant levels of nitrogen to a high-molybdenum stainless steel substantially improve its resistance to pitting in the geothermal environment. For the NRC Division of Reactor Safety Research, the group has been studying the factors causing intergranular stress corrosion cracking of Inconel tubing in PWR steam generators, and has developed a preliminary model predicting the time at which failure can be expected to occur under a variety of conditions. For the NRC's Office of Nuclear Reactor Regulation, BNL has been actively providing technical assistance in the corrosion and stress corrosion areas, and has been performing failure analysis on feedwater nozzles from PWR steam generators, on cracked spent fuel pool piping from Three Mile Island--Unit I, and on turbine rotor discs that have developed stress corrosion cracks in service. On both of the last two investigations, it appears that the sulfur compounds being studied under the basic Energy Sciences Program have played an important role in crack initiation and propagation.

DOE LOW-LEVEL WASTE RESEARCH

A new group has been formed to conduct research for the DOE Low-Level Nuclear Waste Management Program. BNL has been designated as lead laboratory for the development of new low-level waste forms. The program also includes studies of waste segregation practices and experimental evaluation of full-scale radioactive waste forms generated at commercial nuclear power plants.

Other work includes investigation of the leach characteristics of transuranic contaminated incinerator ash waste forms.

FAST-MIXED SPECTRUM REACTOR

The Fast-Mixed Spectrum Reactor (FMSR) is a breeder reactor whose design objective is to provide nuclear energy while at the same time offering excellent proliferation-resistance characteristics. The initial design has evolved into a metal-fueled breeder reactor which employs limited amounts of neutron moderator in certain regions of the reactor core for purposes of reactor safety, control of rate of power change, and also control of local conversion ratios. This design has now been shown to be able to operate on two-year fuel cycles instead of the conventional one-year cycle for its full plant lifetime. The only fuel supplied to this plant over its lifetime subsequent to initial loading is proliferation-resistant natural uranium and all spent fuel may be simply stored and not reprocessed. Reactors of this design are able to produce about four times as much electricity from a given supply of natural uranium as an equivalent common light water reactor.

A new FMSR design was created during the last year. This design is based on the assumption that controlled fuel reprocessing may be acceptable if it is performed only once or twice over the full life of the nuclear reactor. A metal-fueled breeder reactor of the FMSR type designed for these conditions has been shown analytically to have excellent performance, safety, control, and economic characteristics.

National Nuclear Data Center

The National Nuclear Data Center (NNDC) provides services to the entire low energy nuclear science community. The services include information on neutron physics, charged particle reactions, nuclear structure, and decay data.

The IAEA Nuclear Data Section coordinates an international effort in nuclear structure and decay data (NSDD). A network of NSDD evaluation centers has been set up within the United States, and is called the U.S. Nuclear Data Network (USNDN). The USNDN is coordinated by the NNDC which also serves as the United States representative to the international network. The center contributes mass chain evaluations to the Nuclear Data Sheets.

Responsibility for the Nuclear Structure Reference Bibliographic File has been transferred from Oak Ridge National Laboratory to the NNDC. This file is used by the Center to produce the Recent References issue of the Nuclear Data Sheets (Academic Press). The transfer of the Evaluated Nuclear Structure Data File (ENSDF), which is required to produce the remaining issues of the Nuclear Data Sheets, is underway.

The NNDC acts as the secretariat for the Panel on Reference Nuclear Data (formed October, 1976) and hosts the annual meeting of the Panel. The Panel acts as an interface between the scientific community, nuclear data centers, and funding agencies. It advises the centers and agencies of the nuclear data needs of the community and informs the community through the member societies of the data available from the centers. The minutes of the latest Panel issued June 1980 are available as a BNL report. One outgrowth of this Panel has been the annual publication of "A Source List of Nuclear Data Bibliographies, Compilations and Evaluations" compiled, prepared, and disseminated by the NNDC.

The Center released the 4th edition of a bibliography of publications of integral charged particle reaction data, and is continuing its participation in the production of CINDA, a neutron physics bibliography.

The Center acted as host for three important meetings:

Symposium on Neutron Cross Sections From 10-50 MeV, May 12 14, 1980.

Conference on Nuclear Data Evaluation Methods and Procedures, September 22-25, 1980.

Fifth IAEA Consultants' Meeting of Nuclear Reaction Data Centers, September 29-October 3, 1980.

Nuclear Material Safeguards

The function of the Technical Support Organization (TSO) is to provide technical assistance to DOE, NRC, and the Arms Control and Disarmament Agency (ACDA) in their development of policies and procedures in response to perceived threats of sabotage to nuclear facilities and theft or diversion of nuclear material. Internationally, concern centers about the possibility of clandestine production, or national diversion, of material for use in nuclear weapons production (proliferation); domestically, safeguards are aimed at preventing unauthorized possession or use of nuclear materials, and the sabotage of nuclear facilities.

A major emphasis has been continued by the United States in recent years on the need to prevent or delay further nuclear proliferation. The TSO role, under DOE sponsorship, has involved the development of safeguards systems concepts allowing the sensitive and timely detection by the International Atomic Energy Agency (IAEA) of the diversion of nuclear materials or the misuse of a nuclear facility; recent stress has been on gas centrifuge enrichment plants. Also related to the improvement of IAEA capabilities are TSO studies concerning evaluation of safeguards effectiveness and the optimal allocation of IAEA resources; sponsor-

ship is by the U.S. State Department via DOE and the International Safeguards Project Office (ISPO). The "President's Offer" relating to IAEA inspection of U.S. facilities is now in place and TSO has been providing support to both DOE and NRC in implementation. Studies of possible methods to safeguard heavy water and of a specific safeguarding technique of potential use in enrichment plants are being carried out under ACDA sponsorship. Current DOE-funded domestic safeguards studies by TSO involve such areas as consequence analysis, human factors, the compatibility of DOE and NRC safeguards requirements, and the development of a cost effectiveness model to aid in such traditional management decisions as the selection of policy initiatives.

Under NRC sponsorship, a series of studies is being completed on such topics as the effects of licensing reform bills and the technical and legal problems associated with the location and recovery of contraband nuclear material.

INTERNATIONAL SAFEGUARDS PROJECT OFFICE

The U.S. continues to maintain a strong program in support of the IAEA, toward improving the effectiveness of international safeguards. The support program, under technical management of ISPO, is entering its fifth year.

The U.S. Program of Technical Assistance to IAEA Safeguards (POTAS) continues to develop and provide transfer to the IAEA of equipment needed by the IAEA to improve the effectiveness of its Safeguards Program. This (some 34 different types) has included such equipment as assay instrumentation for verification of nuclear material, various types of seals, and video and photographic surveillance systems. Agency data processing and information retrieval have been greatly enhanced by the supply of both computers and programming experts who are cost-free additions to the Agency staff.

An additional effective form of assistance has been provision of cost-free experts for extended service under contract to the IAEA, in the staff of the Division of Development and Technical Support. The contributions by these experts, which to date total 38, have greatly increased the ability of the IAEA safeguards staff to absorb and use the technical improvements which represent the newest developments in both destructive and non-destructive methods of measurement.

POTAS also provides training to members of the IAEA staff and to safeguards personnel of member States, through courses designed to increase the ability of personnel to perform their assigned tasks. Analytical studies have been carried out on pertinent aspects of IAEA safeguards by technical experts, with a view to assessing and improving potential IAEA effectiveness.

ISPO is beginning a new phase of work with IAEA which involves implementing the use in the field of the newly developed equipment and techniques.

In addition, the IAEA has recently identified new tasks where assistance is critically needed. Some of these will be started in 1981.

Advanced Reactor Systems

System studies of processes using fusion energy to produce hydrogen and hydrogen-based synthetic fuels are being carried out by the Department. High temperature electrolysis (HTE) of steam has been identified as the most promising fusion synfuel process. Projected overall efficiencies are in the range of 50 to 70% for conversion of fusion energy to hydrogen chemical energy, depending on process conditions. A unique concept has been developed and extensively analyzed for the extraction of high grade heat (1400°C or higher) by steam cooling of neutron heated, thermally insulated blanket interiors. Experimental tests under simulated blanket conditions have shown that ZrO_2 and Al_2O_3 appear to be suitable materials for high temperature steam cooled blankets. A small demonstration HTE process unit (electrically heated instead of fusion heated) has been constructed to operate at approximately 1000°C for hydrogen production. Tests of electrolyzers have been carried out at 1400°C and promising materials identified.

The Rotating Bed Reactor (RBR) is a compact, very high performance nuclear reactor for space power. Power levels up to several thou-

sand MW(th) can be achieved in a reactor volume of ~1 m^3. Exit temperatures up to ~3000 K are feasible with gas coolants (H_2, He, etc.). Rapid start/stop operation (~1 sec) also appears feasible. Development on the RBR was carried out at BNL during 1965-73 for nuclear space propulsion applications. Extensive thermal-hydraulic tests of rotating fluidized beds were made. These tests demonstrated stable operation under flow conditions comparable to those projected for actual reactors.

More recently, design studies of the RBR have been carried out for space electric power. Pulsed power generation at power levels up to ~1000 MW(e) is achievable with MHD channels. Continuous wave (CW) power generation at levels up to ~100 MW(e) appears achievable using either MHD or high temperature turbines.

DEPARTMENT OF NUCLEAR ENERGY

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Instrumentation Division

Reactor Division

Safety and Environmental Protection Division

Applied Mathematics Department

INTRODUCTION

The Applied Mathematics Department has three missions: to carry out research in the applied mathematical sciences, to provide consultation and professional services in the application of computational, statistical, and mathematical techniques, and to operate and maintain an extensive scientific computational facility.

RESEARCH IN MATHEMATICS

The research in mathematics is concerned with the development and application of analytical and numerical techniques for extracting information from complex mathematical equations arising in energy-related research investigations. The emphasis is on techniques which, although they may be prompted by, and developed in conjunction with, a specific research question, can be expected to have a broad range of application across a number of different programs.

Partial Differential Equations

The major thrust of the mathematical research is on the solution of partial differential equations. Such equations arise in almost every attempt to model theoretically the behavior of a physical object or system. Because of their complexity, approximate numerical techniques must frequently be used to solve them. The main purpose of the research in this area is to understand the nature and reliability of existing approximate methods, and to develop new methods which will reduce the computational effort required to obtain acceptably accurate solutions.

The main emphasis of this work at Brookhaven concerns the solution of important classes of partial differential equations with applications in a wide variety of energy-related areas. This involves (1) analytic investigations of the differential equations and their solutions, (2) the development, analysis, and testing of various algorithms for approximately solving these differential equations, and (3) the application of these results to problems in other areas of research.

The finite element approach has been used as a basis for the analysis and numerical solution of important classes of differential equations. A variable mesh method was applied to elliptic boundary value problems, and the results indicated substantial improvements over approaches using uniform mesh sizes. Iterative algorithms for magnetic field computations were derived and implemented for application to ISABELLE magnet design problems. Several new methods have been developed in response to problems arising in reactor safety research. An advance in calculation of two-phase flow was achieved by demonstrating a new fractional step method. A one-dimensional convergence acceleration technique was developed in collaboration with staff at MIT, and has been applied to reactor safety problems.

Image Reconstruction

Image reconstruction (also called "computerized tomography") is, in general terms, concerned with estimating functions from their integrals over lines or planes in space. This is a topic with a broad range of multidisciplinary applications, and one which has been subject to intensive development since the advent of the first computerized axial tomography (CAT) scanner several years ago. Applied Mathematics Department work in this area has recently been concerned with such problems as (1) establishing general mathematical features, such as the existence of a singular-value decomposition with certain spectral properties, for a particular class of image reconstruction problems; (2) finding consistency conditions for the so-called "attenuated" Radon transform which arises in single-photon emission tomography; (3) reconstruction from projections taken from an arbitrary set of directions; and (4) reconstruction from planar integrals as occur, for example, in nuclear magnetic resonance zeugmatography. Collaborative arrangements have been established with investigators at LBL's Donner Lab,

the U.C. Berkeley Mathematics Department, Ames Laboratory, and the State University of New York at Stony Brook and at Buffalo, as well as collaborative and consultative arrangements with pertinent programs elsewhere at Brookhaven, especially within the Medical Department.

Mathematical Programming

The mathematical programming work is mainly concerned with optimization studies which arise in energy systems analysis. The purpose of the work in these areas is to gain better understanding of existing algorithms and to develop new ones which will allow more complex problems to be attacked with the existing computer technology. The Ho-Manne decomposition algorithm for dynamic linear programs with the staircase structure was implemented in a collaboration with the Center for Operations Research and Econometrics (CORE), Belgium. The computer code (LIFT) is based on the most advanced linear programming software (IBM's MPSX/370) available to date. Together with the previously completed code DECOMPSX for linear programs with the block-angular structure, LIFT extends the capability of MPSX/370 by one hundred fold.

STATISTICAL METHODS

The research in statistical methods is concerned with the mathematics underlying the process of confrontation between measurement or observation, on the one hand, and a theory, model, or expectation, on the other. It involves questions of experimental design as well as those of data analysis and estimation. The mathematical tools to implement objectives in design or analysis do not directly depend on the field of application, and a considerable portion of the work carried out lies in the general area of statistical inference. At the same time, particular fields may raise statistical questions with a specialized focus.

In statistics, the interest is divided between the development and use of new methods, as well as conventional ones to explore new types of problems. A large number of these problems arise in health-related research in the medical and environmental areas, where the fact that the objects under study are human beings leads to considerable restrictions on the manner and extent of data collection.

Work in Mathematical Statistics included Empirical-Bayes methods for estimation of means of normally distributed random variables, adaptive methods in parameter estimation, development of robust statistical procedures, reliability and risk assessment, and sequential experimentation and decision theory.

One of the most attractive applications of such work occurs in the analysis of harmful effects to humans of low dose environmental insults including radioactive and toxic substances. Work has been completed on statistical properties of a generalized model of carcinogenic toxicity. The result allows one to perform low-dose extrapolation for tumors induced by toxic chemicals and/or radiation. A series of studies was carried out to analyze survival when some of the data about the study population is "censored", or missing due to death from causes not under study. The estimators for the regression coefficients were shown to have desirable large sample properties, that is, consistency and asymptotic normality, and furthermore they reduce to the usual least squares estimators when there is no censoring present.

Another area of investigation is likely to have effect on national energy policy. Under a project funded by the U.S. Geological Survey, procedures were developed to obtain statistically meaningful analyses of the internal rates of return of various subpopulations of leases made by the government to the private sector for oil exploration tracts on the outer continental shelf. It is hoped that such analyses will result in greater fairness, higher productivity, and the discouraging of collusion among bidders.

COMPUTER SCIENCE

Computer-related research has focused on two lines of development which will be increasingly important over the next few years. The networking of multiple computer systems is becoming widespread at all levels, from tightly coupled processors exchanging data at high speeds, to loosely coupled geographically distributed networks. Many questions about the optimum way to plan, implement, and operate such networks remain poorly understood. In another direction, the application of computers

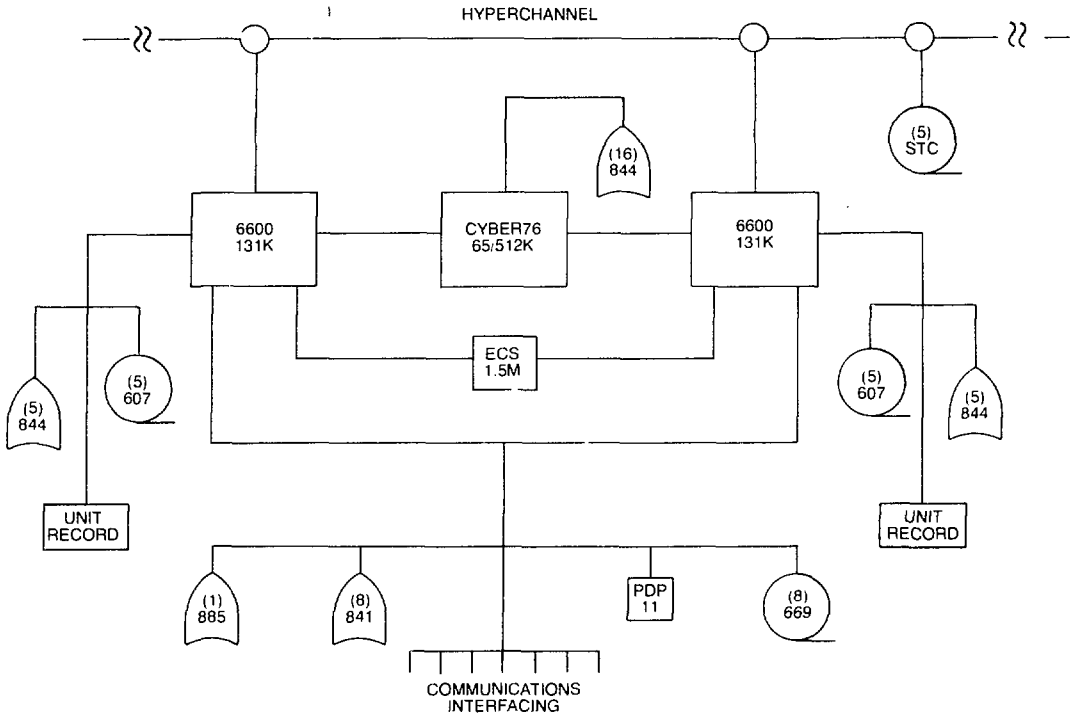


Figure 1. Interconnection of the three major computers and their peripheral equipment within the CSCF. Data communications interfaces are expanded in Fig. 2.

to problems of engineering design, especially of complex digital circuits, is being actively pursued. The current scope of this computer-aided design work includes synthesis, simulation, testability analysis, layout packaging, and documentation of such systems. Work at BNL and elsewhere has demonstrated the feasibility of a unified approach to these diverse problems using a common hardware-description-language data base.

COMPUTING SERVICES

The major part of the Department's resources remains devoted to the Central Scientific Computing Facility. The computing facility, as currently constituted, represents a still-powerful and unique research tool. It is made available to all Brookhaven research programs and to outside collaborators and other government agencies, under special arrangements, through a substantial data communications system. The system is represented in Figs. 1, 2, and 3. These show the interconnection of three large computers, two Control Data 6600s and one CYBER 76, the associated peripherals, their interconnection to a network segment called Hyperchannel, and the data communications subsystem, expanded in Figs. 2 and 3. An important augmentation in service is represented by the procurement of a Large Mass Storage system. This will provide a long-needed expansion of the amount of on-line data storage available to the system. More importantly, it will provide, in addition to its file storage and management capability, a network capability allowing on-line access from a variety of computers at the Laboratory.

The balance of effort between the provision and management of centralized computer facilities and the provision of expert assistance in making use of such facilities is shifting to the

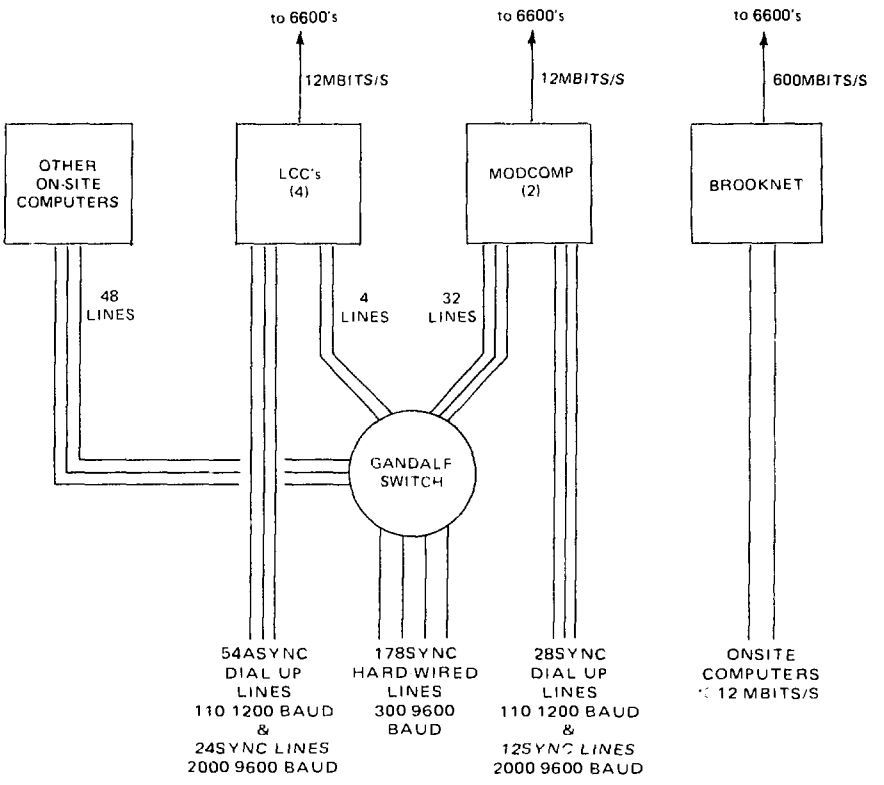


Figure 2. On-site data communications subsystem of the CSCF, showing the varieties of services and switching capabilities offered. These connections extend the resources of the Center to remote areas of the Laboratory as well as to certain off-site locations (see Fig. 3).

latter. For the first time statistical application support is being provided, and more effort is being placed on providing and assisting in the use of high-level software packages. As mini- and micro-computers make more and more powerful computational resources available in association with data acquisition systems or other special purpose computers around the site, the coordination of purchase, maintenance, and systems management will lead to substantial savings and service efficiency.

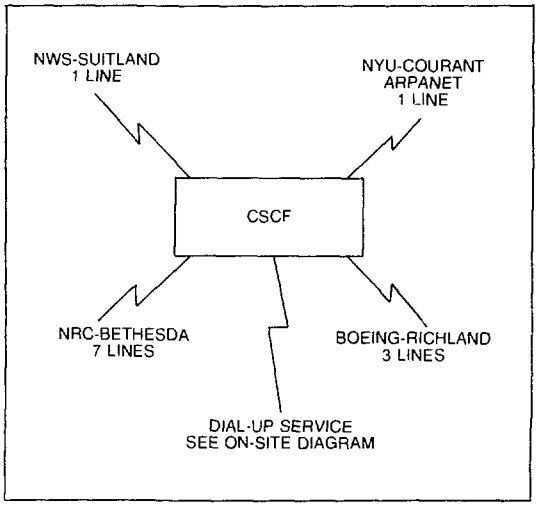


Figure 3. Some of the major off-site data communications links from the CSCF, including those to National Weather Service, Nuclear Regulatory Commission, Richland's Hanford Engineering Labs and the ARPANET national computer network.

Selected Publications

G. H. CAMPBELL, H. E. ROBBINS, and J. YAHAV, Linear and General Empirical Bayes — The Normal Case, submitted to *JASA*.

C. I. GOLDSTEIN, The Finite Element Method With Non-Uniform Mesh Sizes For Unbounded Domains, *Math. of Comput.* (April, 1981).

J. K. HO and E. LOUTE, A Comparative Study of Two Methods For Staircase Linear Programs, *ACM Trans. on Math. Software* **6**, 17-30 (1980).

C. S. KAO, Approximations of Poisson Probabilities, *Proc. ASA 1980 Ann. Meet., Houston, Texas* (August, 1980).

R. B. MARR, C.-N. CHEN and P. C. LAUTERBUR, On Two Approaches to 3D Reconstruction in NMR Zeugmatography, *Proc. Conf. on Math. Aspects of Computerized Tomography,* Mathematisches Forschungsinstitut, Oberwolfach, West Germany (1980).

J. E. PASCIAK, Spectral Methods for Nonlinear Initial Value Problem Involving Pseudo Differential Operators, *SIAM J. Numerical Analysis* (in press).

H. B. STEWART, Fractional Step Methods for Thermohydraulic Calculation, *J. Comput. Phys.* (in press).

J. VANRYZIN and V. SUSARLA, Large Sample Theory for an Estimator of the Mean Survival Time from Censored Samples, *Ann. Stat.*, 8:1001-1016 (1980).

J. VANRYZIN and K. RAI, The Use of Quantal Response Data to Make Predictions, *The Scientific Basis of Toxicity Assessment.* (Ed. H. R. Witschi), 273-290, Elsevier/North-Holland Biomedical Press (1980).

APPLIED MATHEMATICS

R. F. Peierls — Department Chairman
A. M. Peskin — Deputy Chairman
S. S. Rideout — Administrator

G. H. Campbell Computer Science: Distributed computing.

J. E. Denes Head, Central Computer Division.

K. Fuchel Head, Computational Assistance Division.

C. Goldstein, H. B. Stewart, J. Pasciak Partial Differential Equations: Evolution equations, high order stepping methods, elliptic boundary value problems, finite element type methods, multiple fluid flow calculations.

S. Heller Head, Technical Development Division.

J. Ho Optimization and Decision Science: Large scale linear programming, dynamic networks with congestion, multiple criteria optimization, public risk, and individual values.

S. Kao, H. E. Robbins, J. VanRyzin Statistics: Robust test procedures, sequential procedures, empirical Bayes method, and risk analysis.

A. M. Peskin Deputy Chairman and Computer Science: Computer-aided Design.

R. B. Marr Image Reconstruction: Computerized tomography.

Y. Shimamoto Economic rate of return analysis, combinatorial methods.

Instrumentation Division

The Instrumentation Division engages in research and development on recognized problems in scientific instrumentation that are important to the long-term goals of the Laboratory and the Department of Energy. The Division provides consultation services in the areas of instrument specification and selection to other departments of the Laboratory. The Division also designs and constructs some of the instruments required by the departments in the course of their research. These instruments are typically of such an advanced design that they are not commercially available. In addition, the Division provides services in electron microscopy, vacuum technology, printed circuit board fabrication, scientific instrument repair, and computer maintenance.

Members of the Division also collaborate in experiments at BNL and other laboratories when they can contribute significantly to the advance of scientific research with new devices, methods, and techniques developed at BNL.

The principal areas of research activity are the detection of nuclear particles and of radiation with semiconductors and gaseous liquid detectors, processing of signals from detectors, low-noise and other special electronic circuits, systems for acquiring data from, and control of, scientific experiments, and application of nuclear and atomic techniques in elemental analysis and other fields. Some of the more important recent results are described below.

RADIATION DETECTION AND SIGNAL PROCESSING

Position-Sensitive X-ray Detectors

An R&D program on x-ray detectors is being conducted in response to the forthcoming needs at the NSLS where x-ray beams will be used for research on crystal and molecular structures in biology, solid state physics, and chemistry.

For an efficient utilization of the capabilities of the NSLS, the appropriate position-sensitive x-ray photon counting detectors should have properties exceeding the present state of the art, in particular, very high spatial resolution at extreme counting rates. This is required in dynamic (time resolved) studies, e.g., muscle cell contractions where diffraction patterns may have to be obtained in a few milliseconds.

Experimental investigations made here with several small (6×2 cm^2 and 10×2 cm^2) multiwire proportional chambers made for such purposes indicate that a spatial resolution along the anode wires of 100-200 μm could be obtained under total x-ray fluxes of $\sim10^5$ to 10^6 photons/sec without significant deterioration of the spatial resolution or a shift in the position of spectra (Fig. 1). The data rate was limited in these measurements mainly by the electronic signal processing and readout methods. Significant progress in these areas is being made.

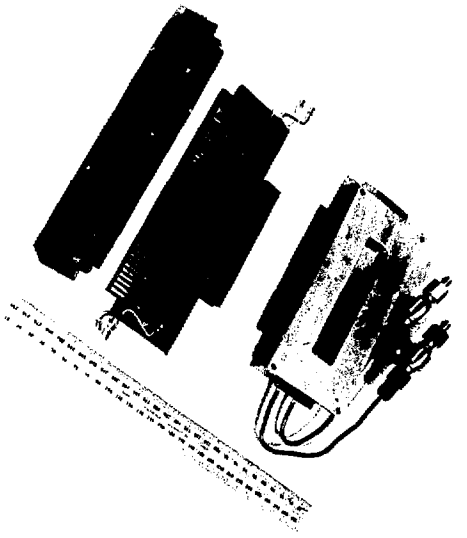


Fig. 1. A view of the detector with one-dimensional position readout by means of a delay line. A 10×2 cm^2 active area detector with Be window is shown with plug-in connections to the delay line. With this detector, a position resolution of better than 200 μm (FWHM) can be obtained. This type of detector will be used extensively for scattering studies of molecular and crystal structures with synchrotron radiation.

Another investigation into the behavior of such chambers at rates of 10^6 to 10^8 counts/sec is being conducted to obtain information on the effects of the space charge due to positive ion

accumulation in the chamber. Smaller avalanche sizes (i.e., lower gas gain) would obviously reduce the space charge. However, with conventional position-readout methods, this would reduce the signal-to-noise ratio and thus increase the spectral line width. The new centroid-finding methods being developed here represent an advance in this area.

Two-Dimensional Neutron Detectors

These detectors are of the multiwire proportional type, employing ^{3}He at 4–6 atmospheres as neutron converter and additional gases for reduction of the range of the interaction products, which limits the spatial resolution. Two 20 × 20 cm^2 chambers with 3 mm FWHM resolution have been in successful use at the HFBR for protein crystal structure studies.

A new 20×20 cm^2 detector, which should represent a substantial improvement in accuracy, has been completed (Fig. 2). It has readout grids near ground potential on each side of the anode plane, and cathodes at negative potential. Multitap connections from the readout grids connect to the centroid-finding position readout system developed here. This system, because of its higher sensitivity, may permit

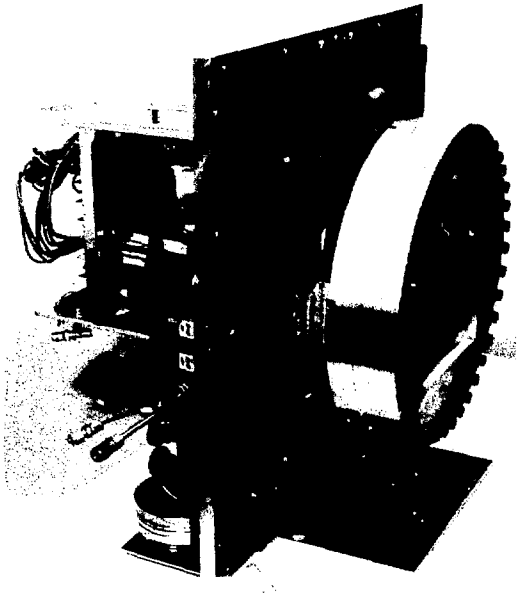


Fig. 2. Two-dimensional position-sensitive detector for thermal neutrons with an active area of 20 × 20 cm^2. In the rear of the detector chamber a part of the centroid-finding position readout system is shown.

introduction of new gas mixtures for improved spatial resolution and for pulse shape discrimination against the γ-ray background. This detector is intended for a small angle scattering facility at the HFBR for use in solid state physics. A larger (50 × 50 cm^2) detector, based on these concepts, is being developed for use in biological research at the HFBR.

Our new centroid-finding method by convolution is being applied to the readout systems for the two large area thermal neutron detectors described above. It makes possible an absolute position accuracy of a few parts in 10^4 of the detector length.

Signal Processing Systems

Utilization of the high luminosity radiation sources which will be provided to experimenters by the NSLS and ISABELLE will require a manyfold improvement in the timing properties and counting rate capabilities of detector readout systems.

Four recently developed readout systems have evolved from studies of the general problem of signal processing at high rates. The centroid-finding method, described here last year, and the delay line readout are being applied to high rate x-ray detectors for use at the NSLS and elsewhere.

Signal processing developments for high energy physics applications include a second coordinate readout for drift chambers, and electronics for particle identification by measurement of the relativistic rise of particle ionization.

Position measurement by determination of the electron drift time in a drift chamber appears to be the most practical way for charged particle momentum measurement in colliding beam experiments. The requirement on the position resolution in the direction of the magnetic deflection (usually azimuthal) is difficult to achieve by any other methods.

The problem arises in determining the second coordinate—along the anode wire. The second coordinate is used to define the angle of the particle track and to establish the consistency of its recognition. Usually a lower accuracy is sufficient for this coordinate.

The feasibility of using an anode wire and surrounding electrodes in drift chambers as a transmission line for second coordinate readout

has been studied. The method is based on propagation of the electromagnetic wave along the anode wire. The position of the avalanche along the anode wire is determined by measurement, in an optimized electronic readout system, of the time difference between the arrivals of the signal at the two ends of the wire. The resolution obtained on long wires (~2 meters) is about 2 cm FWHM for minimum ionizing particles at a gas gain of $\approx 10^5$.

There is increased interest in using gas proportional chambers for particle identification in the relativistic energy range. One of the most promising approaches consists of converting the spatial extent of the ionization into a time sequence. The primary ionization clusters produced by the traversing particle drift toward the anode wire of the chamber, where the gas amplification mechanism results in an electrical signal for each of typically twenty ionization clusters as they arrive at the anode over the course of typically 1 μsec.

A signal processing filter was designed to optimize the reconstruction of the spatial extent of the ionization from the chamber signals. This filter chain consists of a "matched" preamplifier, a shortening filter which effectively cancels the long "tails" of the chamber signals, and a highly symmetric Gaussian integrator. These filters have been applied to preliminary measurements at CERN and on-going ISABELLE detector development experiments at the AGS.

DATA ACQUISITION AND EXPERIMENT CONTROL

National Synchrotron Light Source Motor Control Unit

Many experiments to be performed at the National Synchrotron Light Source will require a VUV or x-ray monochromator and some sort of target-detector spectrometer arrangement. In addition, various other mechanically actuated devices, such as beam defining slits and target sample changers, will be present. For most of these experiments, it will be desirable or even necessary to operate their constituent devices under computer control. (For instance, some devices will reside behind shielding walls and will not be accessible to manual operation while the experiment is in progress.) A widely used and convenient method of implementing mechanical position control is to use stepping motor-position encoder device pairs.

The National Synchrotron Light Source Motor Control Unit is designed to facilitate the operation of monochromators, spectrometers, and other experiment devices having stepping motors as their position changing and holding elements. Communication with the motor control unit is via a full-duplex serial line which conforms to the EIA RS232C interface standard. Thus the complexity of devices which may drive the unit ranges from a simple ASCII terminal to any type and level of computer system which supports an RS232C serial line port (and virtually every computer system does).

The bits transmitted over the serial line are framed into ASCII characters; the characters are grouped together to form words which are recognizable to the human operator. This technique has the advantage that commands to the unit can be generated by typing at an ASCII terminal. A second advantage is that the phrases directed to and returned by the motor control unit can be displayed as ASCII characters so that malfunctions of the unit (or its driving device) become immediately apparent to the human diagnostician.

The motor control unit provides multiple video displays which record all command lines received by the unit and all response lines generated by the unit. These displays also show such parameters as the current position and target position of every axis controlled and the current status of all motor-encoder pairs. A single unit will control as many as fifteen motor-encoder pairs. The unit is designed so that virtually no restrictions are placed on the types of stepping motors or encoders used. The unit is capable of reading both absolute and incremental encoders and employs a serialization technique for reducing the number of cables required between the unit and a high-resolution parallel readout absolute encoder.

A major effort has been made to format the video displays of motor position into types of coordinate system and coordinate system units which are easily recognizable to experimenters. Finally, a manual control box has been provided to allow local (i.e., non-computer) stepping motor control when the user is on the experiment floor.

Currently, five of the motor control units are under construction with their completion

scheduled to coincide with opening of the Light Source x-ray ring.

Oceanographic Instrumentation

The Oceanographic Instrumentation program is based on development of low-power instrumentation for biological and physical measurements in moored systems in continental shelf and slope regions. Measurement sequences, data correlation, storage, and retrieval via stationary satellite telemetry are controlled in each mooring with an array of low-power microprocessor controllers. Synoptic measurements over large shelf areas can be obtained with systems of moorings, each providing time-correlated measurements controlled with arrays of low-power microprocessor controllers. Each mooring will support a number of microprocessor-controlled clusters of biological and physical sensors at appropriate depths.

A single telemetry microprocessor controller in each mooring responds to interrogation from the satellite by interrogating each sensor cluster, in sequence, via serial current loop link for its stored data, then formats the data for satellite transmission, and controls the response to the satellite. A complete microprocessor-controlled system with satellite telemetry controller and two sensor microprocessor arrays based on the RCA-1802 CMOS low power processor has been functioning with extreme reliability during this last year. This system provides the essential basis for future large shelf-area scientific experiments and monitoring.

Data System for Inhalation Toxicology Research Facility

The Inhalation Toxicology Research Facility has been equipped with a data system for the collection, monitoring, and control of experimental equipment and the animal exposure chambers. In addition, the system monitors and processes numerous alarm conditions which are necessary for a safe operation of the Facility. For instance, the temperature, humidity, and the air flow to all the chambers and to the chamber room is being monitored. Approximately 50% of the system is in routine operation. In future implementations the concentrations of the pollutants and exposure will be controlled. The system will also aid in the scheduling of the various activities necessary around the chambers and it will maintain the data of all active experiments on all animals which are under investigation. The fully implemented system will include approximately fifty microprocessors, several million words of semiconductor read/write memory, and numerous UV-erasable read-only memory chips. Thus, the system represents an interesting case of a monitoring and control system architecture allowing extensive use of modern semiconductor device technology.

Distributed Function System Architecture

Studies on the use of large quantities of the emerging inexpensive microprocessors and associated Very Large Scale Integration (VLSI) chips within integrated distributed function control and data acquisition system architectures have been pursued in the past several years. Some systems developed in the early 1970's have been implemented using minicomputers in places where inexpensive microprocessors have been anticipated in future applications. Between 1977 and 1979, an approach was developed for the implementation of such systems and some key elements were implemented and demonstrated. A recently completed study for the ISABELLE control system is based on this approach.[1] The traditional partitioning of a system, the "host" computer, several "satellite" computers, the interface, and the front-end, has been eliminated in favor of more appropriate arrangements. Hardware and software are grouped into nodes, where one or several nodes are assigned to a complete function, such as file management, communication, general execution, sensor service, or software development. Several nodes are grouped into a cluster. The nodes communicate via a cluster memory in-line with processor instructions. Several clusters are grouped into a system. For intercluster communication, a long-distance communication subsystem with associated controllers based on a frequency modulation concept has been developed. This subsystem has a bandwidth of 1 MHz, using inexpensive VLSI chips and coaxial cables available from the commercial television technology. There are no systematic limitations on the size of the system and the

interconnection complexity of the various clusters.

Monitoring System for Superconducting Power Transmission Line Test Facility

A computer system has been developed for real-time data acquisition and monitoring of the 100-meter Superconducting Transmission Line Test Facility of the Accelerator Department. Functionally distributed, independent processors handle command entry, data collection, parametric conversion, CRT data display, and alarm warnings. A shared memory enables inter-processor communication and storage for data base and data file structures. The system has successfully functioned during cool-down tests of the Transmission Line Facility. In addition, an independent minicomputer station has been developed to support user program development and data analysis.

NUCLEAR ANALYTIC TECHNIQUES AND SEMICONDUCTOR TECHNOLOGY

Radiation Damage in Silicon Surface Barrier Detectors

During the past twenty years of use of silicon surface barrier or junction detectors for energetic charged particles, relatively little has been understood about the basic mechanisms of radiation damage, particularly that caused by fast neutrons, a common background in accelerator experiments. Moreover, little agreement exists on the specific mode or rate of failure in a given radiation field. Further study of radiation damage in silicon detectors has been stimulated by their potential application as position-sensitive detectors in both colliding beam and fixed target experiments in high energy physics, where reasonable predictions of useful detector lifetime are required. Radiation damage may result from primary protons or other minimum-ionizing particles or from background neutrons.

Radiation damage has been studied intensively but somewhat empirically by silicon device technologists who have independently accumulated data on the effect of several radiation fields, including fast neutrons, on parameters of mutual interest such as carrier lifetime degradation and leakage current. Experimental data have been interpreted by a linear relationship of effect to fluence with the proportionality constant called, appropriately, the damage constant. Damage constants derived from silicon device studies (e.g., MOS devices) have become useful to radiation detector damage studies, in part because they represent the only substantial data available and also because it has been found that reasonable agreement between the two regimes apparently exists.

Several totally depleted silicon surface barrier detectors were irradiated with high energy protons near a production target in the test beam at the AGS.[2] The detectors quickly developed higher leakage currents and worsened charge collection properties and it was concluded that a very high fast-neutron background component was responsible. Activation samples substantiated this conclusion and placed the fast neutron fluence at the detector position at the 10^{14} n/cm^2 level, where silicon device damage constants predict the observed leakage current behavior. Other effects, such as semiconductor type change and base resistivity increase, were also observed and were consistent with other damage experience.

The radiation environment of this experiment is believed to be vastly different from that of a colliding beam experiment and this hypothesis was tested by exposures of both silicon detectors and activation samples at the ISR at CERN. To date, a very low fast-neutron background has been observed, and little effect on the detectors has been noted for short initial exposures.

References

[1] D. GERD DIMMLER, Results of an R&D Effort on the ISABELLE Control System; BNL 25528, (May 1979).

[2] H. W. KRANER, T. LUDLAM, D. KRAUS and J. RENARDY, Radiation Damage in Silicon Surface Barrier Detectors, BNL 28311; presented at the conference on "Miniaturization of High Energy Physics Detectors", University of Pisa, Pisa, Italy, 18-20 September (1980); to be published in the Proceedings of this conference.

Selected Publications

1. H. W. KRANER, Fast Neutron Damage in Germanium Detectors, *IEEE Trans. Nucl. Sci.* **NS-27,** 218-234 (1980).

2. R. A. BOIE AND V. RADEKA, High Precision Position Readout for Large Area Neutron Detectors, *IEEE Trans. Nucl. Sci.* **NS-27,** 338-350 (1980).

3. EMILIO GATTI, HIDEKI OKUNO, AND MARINA ARTUSO, Interwoven Grid Wires for Second Coordinate Readout in MWPC, *Nucl. Instr. & Meth.* **167,** 417-422 (1979).

4. VELJKO RADEKA AND ROBERT A. BOIE, Centroid Finding Method for Position-Sensitive Detectors *Nucl. Instr. & Meth.* **178,** 543-554 (1980).

5. K. J. ELLIS, D. VARTSKY, T. B. PEARLSTEIN, J. L. ALBERI, AND S. H. COHN, A Dual-Photon Absorptiometer Utilizing a HpGe Detector and Microprocessor Controller, *Proc. 4th Int. Conf. on Bone Measurement,* NIH Publication No. 80-1938, 1-8 (May 1980).

6. A. H. WALENTA, Performance and Development of dE/dx Counters, BNL 28328, presented at Int. Conf. on Experimentation at LEP, Uppsala, Sweden, (June 16-20 1980), *Physica Scripta,* **23,** 353 (1981).

7. H. W. KRANER AND K. W. JONES, Application of Nuclear Microlocalization to Biomedical Problems, BNL 28573; presented at Conf. on Application of Accelerators in Research and Industry, Denton, Texas, (November 3-5 1980), *IEEE Trans. Nucl. Sci.,* **NS-28,** 1424-28 (1981).

8. J. L. ALBERI AND F. W. STUBBLEFIELD, A Spectrometer Control Subsystem with High Level Functionality for Use at the National Synchrotron Light Source, BNL 28583, *IEEE Trans. Nucl. Sci.* **NS-28,** 351-358 (1981).

9. R. A. BOIE, V. RADEKA, P. REHAK, AND D. M. XI, Second Coordinate Readout in Drift Chambers by Timing of the Electromagnetic Wave Propagating Along the Anode Wire, BNL 28660, *IEEE Trans. Nucl. Sci.* **NS-28,** 471-477 (1981).

10. R. A. BOIE, A. T. HRISOHO, AND P. REHAK, Signal Shaping and Tail Cancellation for Gas Proportional Detectors at High Counting Rates, BNL 28691, *IEEE Trans. Nucl. Sci.* **NS-28,** 603-609 (1981).

INSTRUMENTATION DIVISION

V. Radeka, Head

J. L. Alberi Development of data acquisition and experiment control systems
R. A. Boie Signal processing electronics and detector readout systems
R. P. DiNardo Electrical and optical coatings, detector fabrication, and specialized materials processing
D. G. Dimmler Control and data acquisition system architectures, microprocessor applications, and oceanographic instrumentation
J. Fischer Physics of radiation and particle detectors, applications of detectors in physics, chemistry, and biology
N. E. Greenlaw Data acquisition and experiment control systems software
Y. Inagaki* Physics of radiation and particle detectors, applications of detectors in physics, chemistry, and biology
M. A. Kelley Data acquisition and experiment control systems software
H. W. Kraner Nuclear analytic techniques and semiconductor technology
G. P. Larson Development of data acquisition and experiment control systems
D. W. Potter Laboratory instrumentation, Radio Communications Officer
V. Radeka Signal processing and noise in physical measurements; detectors and electronics
S. Rankowitz Systems, electronics, and oceanographic instrumentation
L. C. Rogers Signal processing electronics and low background counting systems
G. F. Sintchak Pulse height analyzers, computer-based instrumentation, biomedical electronics, RF system design
F. W. Stubblefield Multi-processor operating systems, high-speed data acquisition electronics and computer interfaces, medical electronics for flow microfluorometry
P. Z. Takacs Optical metrology and instrument design for synchrotron radiation applications
A. H. Walenta Studies of the physics of advanced ionization detectors, applications of such detectors to particle physics, solid state physics, biology and medicine
J. B. Warren Analytical electron microscopy, including SEM, EDX, microdiffraction, and computer simulation of crystal defect images

*Kyoto University, Kyoto, Japan

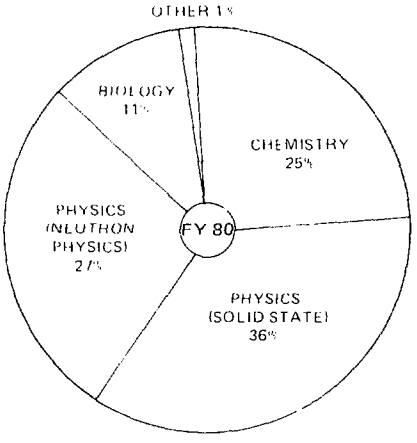
Reactor Division

The Reactor Division is charged with the responsibility of operating BNL's two nuclear reactors in a safe and economical manner while providing neutrons used in beam experiments and for the irradiation of specimens. The High Flux Beam Reactor (HFBR) produced approximately 8400 megawatt days of integrated thermal energy during the past year. There were 11 unscheduled interruptions, amounting to 2.9% unscheduled reactor downtime overall. The Brookhaven Medical Research Reactor (BMRR) was run only upon demand, and produced 359 megawatt hours of energy during the past year, an increase of 33% over the previous year.

Table I shows the distribution of the support of HFBR Operations from the scientific programs, and Table II lists the service irradiations performed.

TABLE I

Distribution of Support of HFBR Operations From Scientific Programs



	USE CHARGES FISCAL YEAR 1980	
	AMOUNT $	% OF SUPPORT
Physics Department		
Neutron Physics	720,361	27
Solid State Physics	960,481	36
Biology Department		
Analysis of Biological Structures	293,480	11
Chemistry Department		
Molecular Chemistry	667,000	25
Other		
Energy and Environment Department		
Irradiation Services	26,680	1
Total	2,668,002	100

TABLE II

Reactor Service Irradiations

Organization	HFBR	BMRR
Chemistry Department	180	9
Department of Energy and Environment	17	0
Department of Nuclear Energy	5	0
Medical Department	4	37
Physics Department	4	1
Reactor Division	9	4
Safety and Environmental Protection Division	0	9
Outside Organizations	27	52
Total	246	112

HFBR Improvements and Modifications

During 1980, new heat exchangers were installed in the HFBR cooling system, which will permit operation at a 50% higher power level than the present 40 megawatts. It is expected that all of the necessary extensive safety reviews will be completed during the first half of 1981, and operation at 60 megawatts will begin towards the end of the year.

Cold neutrons were obtained for the first time from the Cold Neutron Facility during 1980. This facility increases the available intensity of low energy neutrons (having wavelengths greater than 4 angstroms) by a factor 5 to 10. After some necessary design modifications were made, the facility became available for routine operation in experiments early in 1981.

TRISTAN II, an on-line isotope separator for the study of neutron-rich unstable isotopes produced from ^{235}U fission, has been operating successfully since its installation last year. The beam intensity obtained from this device has exceeded design expectations, giving a flux of these isotopes which is nearly a factor 10 higher than that available anywhere else in the world at this time.

REACTOR DIVISION

G. C. Kinne, Division Manager
D. Rorer, Deputy Division Manager *

High Flux Beam Reactor Operations
M. Brooks, Group Leader
D. Oldham, Asst. Group Leader
R. Bergoffen, Reactor Supervisor

Reactor Instrument Group
D. G. Pitcher, Group Leader
S. Moss, Instrument Engineer

Reactor Maintenance Group
M. Zukas, Group Leader

Research Coordination Group
D. Rorer, Group Leader *

Water Chemistry
S. Protter, Group Leader

Reactor Technical Assistance
P. Tichler, Chemical Engineer
K. Y. Cheung, Nuclear Engineer

Quality Assurance Office
J. Detweiler, Coordinator *

Medical Research Reactor Operations
J. Detweiler, Supervisor *

Training & Procedures Office
J. Phillips, Coordinator

Source & Special Nuclear Materials Group
P. Colsmann, Group Leader
K. Dahms, Engineer

Reactor Special Projects
R. Karol, Coordinator

Doe Standards Group
W. Brynda, Group Leader
L.L. Junker, Project Engineer

*More than one position

Safety and Environmental Protection Division

INTRODUCTION

The Safety and Environmental Protection Division provides technical and professional services in areas of health and safety. It also carries on basic and applied research in these areas. Its health and safety services include: professional consultation, guidance, and review of safety aspects of new facilities or programs; sampling, analysis, and evaluation of potentially hazardous operations already in existence; development of safety guides; waste management; also training in industrial safety, cardiopulmonary resuscitation, respirator use, health physics, industrial hygiene, fork truck and crane safety, and emergency response. The Division's fire-rescue and police groups play key roles in ensuring that the Laboratory can cope effectively with local emergencies.

The Division is responsible for several research programs which relate to the evaluation of potential health and safety hazards of energy sources or byproducts. These programs include two directed at evaluation of the past and anticipated future ionizing radiation dose equivalents to residents of the Marshall Islands; two which involve studies of basic quantities in radiological physics and their relationship to biological effects of ionizing radiation and other agents having carcinogenic or mutagenic potential; two in the area of assessment of hazards and development of protection guidelines for chemical and physical hazards; one in which genetic effects of energy-related agents, e.g., strong magnetic fields and ionizing radiation, are studied; and one which provides practical field training and research experience for graduate students in radiological and environmental sciences.

MUTAGENIC EFFECTS OF POLLUTANTS

Possible induction of recessive lethal mutations in stem cell spermatogonia of *Drosophila* was studied. Mutations in these cells are especially important since they continue to divide throughout the organism's life and produce cells which develop into sperm. Embryonic stages (which contain only the primary stem cell type spermatogonial cells) were studied by exposing *Drosophila* eggs to gaseous ethylene dibromide at various concentrations. Spermatogonial mutations were induced in large numbers and a dose-response relation was observed. In one of these experiments, the males treated as embryos were brooded daily for several days to investigate the sensitivity of stem cell spermatogonia. A few of these males, treated as developing embryos, continued to produce a large number of mutations for all the tested days suggesting a mutation induction in one of the five or six stem cell spermatogonia. As far as we are aware, this is the first evidence of chemically induced mutation in the stem cell spermatogonia. These observations have an important bearing on the safety limits being prepared for this widely used chemical.

TOXIC MATERIAL ADVISORY PROGRAM

The Toxic Material Advisory Program continues to provide the basic foundation to develop interim exposure guidelines, work practices, and consultation in the functional areas of toxicology, physiology, biological monitoring, workplace sampling, health assessment methodologies, risk assessment, and hazard analysis. Initially, the Center for Assessment of Chemical and Physical Hazards (CACPH) had been established within the Safety and Environmental Protection Division to facilitate the timely development of interim standards for potential occupational and environmental hazards that may be associated with activities of the Department of Energy. At CACPH particular emphasis is directed toward the development and eventual promulgation of interim standards for those energy technologies having high probability of commercialization. Key factors associated with the establishment of this support program are flexibility and the ability to re-

spond to changing problems with multidisciplinary expertise. Currently CACPH also serves to provide comprehensive industrial hygiene assistance to DOE's Operational and Environmental Safety Division in its prime responsibility of supporting the environmental activities of the developing energy technology programs.

Fiscal year 1980 accomplishments include the following:
Toxic Material Advisory Report for 2-Mercaptoethanol, Draft Toxic Material Advisory Report for Acetylacetone, Health Hazard Assessment Summary Report on Beryllium Silicon Nitride Ceramics, Industrial Hygiene Consultation Report for the Western Area Power Authority, and Industrial Hygiene Consultation Report on Wood Preservation Practices with Pentachlorophenol.

Other activities include review and technical support for the Industrial Hygiene/Epidemiology Study of the Commercial Lurgi Gasification Plant in Kosovo, Yugoslavia, and technical assistance in the development of a DOE carcinogen policy. The program manager provided technical assistance as part of a four member U.S. team visiting the various technical institutes in Yugoslavia that will be participating in the study.

MARSHALL ISLANDS STUDIES[1,2,3]

A field trip was undertaken to Japtan and Enewetak Islands, Enewetak Atoll, and Ujelang Island, Ujelang Atoll, to obtain baseline body burden data on the Enewetak population prior to the repatriation of Enewetak Atoll in April, 1980. Another field trip was undertaken to Majuro Atoll and Kili Island for whole-body counting of former Bikini residents and a comparison population. Consecutive measurements of a Bikini resident's body burden post departure allowed computation of individual long term biological removal rate constants. Human milk samples were obtained from four lactating former Bikini adult females, whose ^{137}Cs body burdens had been defined by whole-body counting and radiochemical analysis of urine samples. Results were used to estimate the dose equivalent to infants whose primary food supply was human milk and coconut tree products. Dose-equivalent commitments were estimated for adults who may return to Enue Island, Bikini Atoll. This calculation was based on ^{137}Cs activity transfer factors derived from review of whole-body counting data and analyses of coconut tree products.

Retrospective and contemporary external exposure rate data, whole-body counting data, and radiochemical analyses of urine data were reviewed for the interval June, 1954, to December, 1980, for the Utirikese and from June, 1957, to December, 1980, for the Rongelapese. An example of internal dose-equivalent rates for the total body is presented in Fig. 1 for the

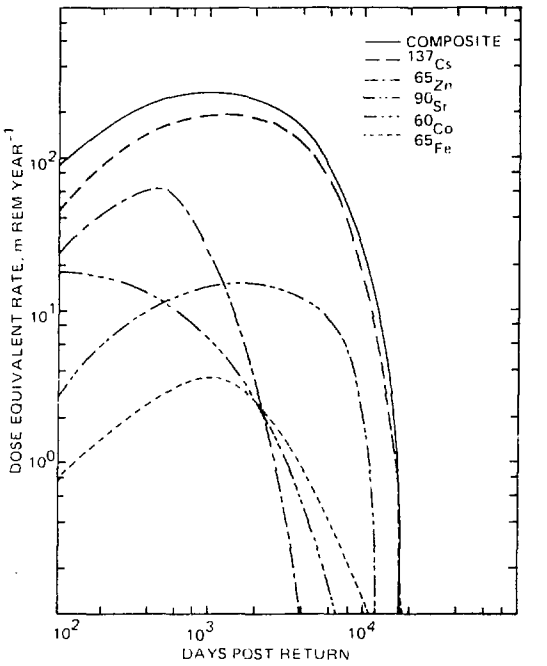


Figure 1. Adult mean total body dose-equivalent rate at Rongelap Atoll post mid-1957.

Rongelapese adults. Dosimetric models which best describe the declining continuous uptake regime were constructed for the nuclides of interest. Daily activity ingestion rates, total body dose-equivalent rates, and dose-equivalent commitments to various organs were determined for population subgroups and for individuals.

An acute dose reassessment from Castle Bravo fallout is being made using three independent approaches based on: 1) biological

samples from the evacuated Rongelap population, 2) historical soil samples, and 3) weather data obtained during the test at Bikini Atoll. Additionally, a study of diet and living patterns among the inhabitants of the Northern Marshall Islands has been drafted. This information is used as input for accurate assessment of chronic internal and external dose-equivalent commitments.

RADIOLOGICAL RESEARCH ACCELERATOR FACILITY

During the first six months of the past year, the Radiological Research Accelerator Facility continued to operate as a national facility for radiobiology using high-LET radiations. The last half of the year was spent disassembling, packing, and shipping the facility to Nevis Laboratories of Columbia University for future use there. The facility was very heavily used during January to March in order to satisfactorily complete the five experiments conducted by outside users, six by BNL users, and six by users from the Radiological Research Laboratory of Columbia University. The radiation induced biological effects studied include mutation in *Drosophila melanogaster*, late effects in rat fetuses irradiated *in utero*, oocyte death in newborn and *in utero* mice, and transformation of C3H 10T½ mouse cells to a malignant state. Cell survival after irradiations with neutrons and mixed high-LET radiation and x-ray irradiation was studied with mouse, Chinese hamster V79, and human T-1 cells. A technique for noninvasively measuring the silicon content of human lungs was developed. The program is now dormant for at least one more year while the facility is being reestablished and restaffed at Nevis Laboratories in Irvington, NY.

References

1. R. P. MILTENBERGER, E. T. LESSARD, and N. A. GREENHOUSE. ^{60}Co and ^{137}Cs Long Term Biological Removal Rate Constants for the Marshallese Population. *Health Physics*, **40**, 615-23, (1981).

2. E. T. LESSARD, N. A. GREENHOUSE, and R. P. MILTENBERGER. A Reconstruction of Chronic Dose Equivalents for Rongelap and Utirik Residents—1954-1980. BNL 51257, October, 1980.

3. R. P. MILTENBERGER, N. A. GREENHOUSE, and E. T. LESSARD. Whole Body Counting Results from 1974 to 1979 for Bikini Island Residents. *Health Physics* **39**, 395-407, (1980).

SAFETY AND ENVIRONMENTAL PROTECTION DIVISION

C.B. Meinhold, Division Head
W.R. Casey, Deputy Division Head
J.W. Baum, Research Coordinator
R.W. Young, Security Officer

*R. S. Baloyi	Industrial Hygiene
J. W. Baum	Radiological Physics, Health Risk Assessments
P. R. Becker	Safety Engineering, Marine Safety
N. M. Bernholc	Industrial Hygiene
B. F. Brennan	Plant Protection
J. B. Deitz	Fire Protection Engineering
†C. H. Distenfeld	Health Physics, Instrumentation, Emergency Planning
P. G. Edwards	Hazardous Waste Management
N. J. Fallon	Computer Science
C. W. Flood	Health Physics, Emergency Planning
‡N. A. Greenhouse	Marshall Islands, Health Physics
A. P. Hull	Environmental Monitoring, Health Physics
A. F. Humm	Health Physics
H. M. Kalbach	Administration
P. Kale	Mutagenesis
D. Kirson	Fire Protection Engineering
G. L. Krieger	Health Physics
A. V. Kuehner	Computer Science, Radiological Physics
E. T. Lessard	Marshall Islands
**G. S. Levine	Electronics, Health Physics
S. A. Marino	Radiological Physics, Accelerator Physics
R. J. McWilliams	Safety Engineering, Construction Safety
R. E. Mills	Radiological Physics, Dosimetry
R. P. Mittenberger	Marshall Islands, Internal Dosimetry
A. R. Moorthy	Radiochemistry
J. R. Naidu	Environmental Studies, Ecology
M. P. O'Brien	Training
S. G. Pearsall	Safety Engineering, First Aid, Training
L. F. Phillips	Personnel Dosimetry, Health Physics, Calibrations
A. P. Porteous	Mutagenesis
N. D. Rohrig	Radiological Physics, Accelerator Physics
H. Schulman	Safety Engineering, Pressure Systems
J. J. Shonka	Health Physics, Radiological Physics
B. D. Silverstein	Industrial Hygiene
J. R. Steimers	Analytical Chemistry
C. F. Swezey	Personnel Monitoring
M. N. Varma	Dosimetry Research, Surface Physics, Radiological Physics
G. N. Wall	Electrical Safety, Safety Engineering
O. White	Industrial Hygiene
R. Young	Safety Engineering, Security

*Terminated July 1980
†Terminated August 1980
‡Terminated September 1980
**Transferred to Dept. Nucl. Eng., April 1980

7

General and Administrative

General and Administrative

PERSONNEL STATISTICS

As shown in Table I, growth in the Laboratory work force has continued the slowing trend noted in the last several years. Growth in 1978 was 7.3%, in 1979, 3.1%, and in 1980, 1.9%. This trend reflects the slowdown in staffing of the two new major research facilities, ISABELLE and the National Synchrotron Light Source, and in the energy sciences areas.

Table II shows some growth taking place in the scientific staff. The scientific staff total increased 7.8% in 1978, 0.8% in 1979, and 4.5% in 1980.

Table III indicates a substantial growth in the summer program, up 8% over the previous year. This reverses the downward trend noted in the past three years.

On the other hand, scientific guest and collaborator appointments (Table IV) were down by 1.4%. Table V shows a mixed trend, there were more consultant contracts in effect than in FY 1979, and more consultants were used, but the number of man-days declined 8.3%.

Table I
Employment Statistics

	Sept. 30, 1980	Sept. 30, 1979	Sept. 30, 1978
Scientific staff[a]	783	765	763
Scientific professional staff	571	560	526
Nonscientific staff[b]	2281	2242	2170
Total	3635	3567	3459

Turnover Data

	1980		1979		1978	
	Number	Annual rate(%)	Number	Annual rate(%)	Number	Annual rate(%)
Accessions						
Scientific staff[a]	111	14	126	17	173	23
Scientific professional staff	87	15	107	19	135	26
Nonscientific staff[b]	210	9	238	11	310	14
Total	408	11	471	13	618	18
Separations						
Scientific staff[a]	98	13	102	13	135	18
Scientific professional staff	86	15	82	15	78	15
Nonscientific staff[b]	201	9	178	8	199	9
Total	385	11	362	10	412	12
Net Accessions						
Scientific staff[a]	13	2	24	3	38	5
Scientific professional staff	1	—	25	5	57	11
Nonscientific staff[b]	9	—	60	3	111	5
Total	23	1	109	3	206	6

[a]Includes Research Associates and Visitors.
[b]Figures do not include temporary summer nonstudent employees. Temporary student employees are included in Table III.

Table II

Scientific Staff and Students on June 30

	Regular Staff			Salaried Visitors		
	1980	1979	1978	1980	1979	1978
By appointment category						
Staff						
Senior Scientist	111	107	123	1	1	2
Scientist	294	272	255	19	11	11
Associate Scientist	159	169	162	13	8	8
Assistant Scientist	93	81	84	9	1	3
Senior Research Associate	—	—	—	9	11	12
Research Associate	—	—	—	55	69	72
Students						
Junior Research Associate	—	—	—	8	12	10
Research Assistant	—	—	—	—	3	—
Total	657	629	624	114	116	118
By academic degree						
Ph.D. or M.D.	542	523	513	97	97	114
Master	45	42	46	12	11	3
Bachelor	65	59	61	4	8	1
No degree	5	5	4	1	—	—

Table III

Summer Program 1980

	Staff	Students[a]	Salaried	Unsalaried	Institutions
By department					
Accelerator	16	9	7	18	16
Applied Math	6	1	4	3	4
Biology	15	3	4	14	12
Chemistry	14	5	4	15	11
Directors' Office	1	2	0	3	3
Energy & Environment	26	24	15	35	13
Instrumentation	1	1	1	1	2
Medical	12	14	1	25	21
Nuclear Energy	9	7	9	7	12
Physics	109	15	38	86	65
SEPD	1	16	1	16	9
Total	210	97	84	223	

[a]Includes 69 Participants in Summer Student Program for 1980.

AFFIRMATIVE ACTION

A representative breakdown of ethnic minorities and of women for the period between October 1, 1979, and September 30, 1980, is presented in Table VI. Minorities increased 3.86% and Women 2.1% during this period.

The Laboratory completed its first year of participation in the National Consortium for Graduate Degrees for Minorities in Engineering (GEM). Four Black students participated in the program.

Three student engineers will participate in the program during the summer of 1981.

A Day Care/Learning Center was established by Educational Research Consultants at a location in proximity to the Laboratory. The Center began operations in late summer and has an enrollment which is largely composed of children of Laboratory employees.

The Executive Office of the President, Office of Science and Technology funded a program of apprenticeships for minority high school students to be conducted at the national research laboratories.

The program objective was to stimulate a broader interest and awareness among minority students in science and technical careers. Thirty minority students participated in this program.

Table IV

Scientific Guest and Collaborator Appointments (Unsalaried) in effect on Sept. 30, 1980

By department	
Accelerator	31
Applied Mathematics	3
Biology	70
Chemistry	157
Energy and Environment	77
Instrumentation	8
Medical	251
Nuclear Energy	7
Physics	764
Reactor	36
Safety and Environmental Protection	41
Total	1445

[a]Represents 289 institutions, including 73 outside the United States.

Table V

Consultant Services

	1980 Fiscal year
Total contracts in effect	386
No. of consultants used	234
No. of man-days of service	5,497.76

Table VI

Minority Employees

	10/1/79		9/30/80	
Category	Total	%	Total	%
Minority	492	13.8	511	14.1
Black	248	7.0	258	7.1
Hispanic	79	2.2	83	2.3
Amer. Indian/ Alaskan Native	12	0.3	13	0.4
Asian/Pacific Islander	153	4.3	157	4.3
Women	760	21.3	776	21.3
Laboratory Total	3567	100.0	3635	100.0

ADMINISTRATION

On October 1, 1979, Mary Winkels became Manager of the Technical Information Division, replacing John P. Binnington who retired.

On October 15, Dr. Richard B. Setlow became Chairman of the Biology Department for a five-year term, replacing Dr. Elliott N. Shaw.

Effective January 1, 1980, Robert W. Young, of the Safety and Environmental Protection Division, was appointed Laboratory Security Officer.

On February 1, Gerald C. Kinne replaced Robert W. Powell as Head of the Reactor Division. Mr. Powell, who retired on February 29, joined the Laboratory in 1947 and was instrumental in the development and operation of all three of the Brookhaven research reactors.

On September 1, John Laurie became Manager of the Photography and Graphic Arts Division.

On September 17, Dr. Kjell Johnsen became Technical Director of the ISABELLE Project, in addition to his duties as Deputy Head. Dr. James Sanford, Head of the Project, retains direct responsibility for the Conventional Construction, Experimental Areas, and Detector Divisions, as well as overall administration of the Project.

SERVICE ORGANIZATIONS

Division of Contracts and Procurement

During the fiscal year the Division of Contracts & Procurement negotiated over $1,400,000 in savings for the Laboratory.

The division handled 34,000 transactions totalling more than $80,000,000; a significant increase in dollars. Included in these figures was $22,000,000 spent with 1300 local firms, an increase of 22% over the prior fiscal year.

Fiscal Division

The installation of an inquiry terminal in Payroll for the accessing of data has been most

helpful. Expansion of the inquiry system is expected to apply to other systems in the future.

The new Accounts Receivable System is in the developmental stage. We anticipate this will be operational in FY 81.

Photography and Graphic Arts Division

In July, DOE approval was received for the acquisition of electronic typesetting equipment. This more modern and versatile technology will replace our existing antiquated machines and thus reduce publishing costs to the Laboratory.

After nearly 21 years of operation, the High Speed Film Processing operation within Photography has been phased out. This operation processed film which was generated by the Brookhaven Bubble Chambers.

A full time graphic analyst was hired within the Micrographics group. This will give us the necessary technical support to enable the Laboratory to more effectively make use of the utility publication capability of our COM (Computer Output Microfilm) device.

Plant Engineering

One innovation in the Electrical Division has been increased use of the computer for power billing and rate analysis. Breakdown of power costs by buildings, which formally required a half-day's work, is now accomplished in 15 minutes using a self-developed program and a remote computer terminal. This becomes increasingly important as preparations are made for billing each department for its power use. Another computer program has been a valuable tool in analysing LILCO's proposed contract changes. Because of the tremendous impact of high power costs on BNL operations, increased time has been devoted to analysis and prediction of LILCO rates.

Continued use of alternate liquid fuels enabled BNL to save $743,000.

The insulation system, developed at BNL, was written up in several publications resulting in over one hundred inquiries for additional information. The system was recently used to insulate the masonry walls of the Research Library. A Conservation of Energy funding request has been submitted which, if approved, will provide for insulating several major masonry buildings on site.

STAFF SERVICES DIVISION

New Telephone System

A contract was signed with General Telephone and Electronics/Automatic Electric for a new leased telephone system. Operational procedures, installation guidelines, and a cutover schedule were established early in FY 80.

There have been no major delays in the progress of work that would postpone the April 3, 1981 project completion date. Cable, the telephone switch, and telephone equipment have been delivered on schedule.

Initial data base information for the computerized telephone switch and preliminary individual telephone station requirement design have been completed. Lengthy negotiations with GTE resulted in a significant reduction in cost for *new* work on the outside cable plant.

DECAT

A new program here at BNL, Driver Energy Conservation Awareness Training (DECAT) was implemented in October of this year. It is sponsored by the DOE and was developed by Reynolds Electrical & Engineering Co., Inc., a prime contractor to the DOE. It emphasizes what managers of large fleets as well as individual operators can do to stretch their gasoline dollars through more fuel-efficient practices without impairing or sacrificing transportation resources. It also has been implemented at other government and private facilities through which DOE is encouraging energy conservation on our nation's highways.

Supply and Material

Greater emphasis has been placed on the rehabilitation of existing office furniture as a means of reducing procurement requirements for new furniture. We have established a contract for these services and as equipment is refurbished, we are establishing new stock items at substantially lower unit prices. The Laboratory took part in the closing of a Government facility, Frankfort Arsenal, in Philadelphia, and we were able to acquire 298 various style office chairs.

Within the Excess Property network we found that a DOE Pool existed for the supply of lead. The lead is available to DOE contractors on a non-reimbursable basis and, to date, we have filled two requirements resulting in a savings of $18,000.

Improvements have been made in the use of the Bill of Materials concept for the various trade groups and a separate storage facility has been completed. The new facility is located adjacent to Building T-91 and consists of two renovated house trailers. We will continue to support and expand this program in the coming fiscal year.

Technical Information Division

A program was written which enables us to utilize relevant information from TIC magnetic tapes available from NTIS. These tapes provide bibliographic data for all reports received on standard distribution. Creative utilization of available information in this manner automates report activity on site, creating a union list of holdings on-line and providing input capabilities for all libraries, plus access through any remote location terminal capable of dial-up contact with the CDC 6600.

Attendant benefits are: minimal keyboarding for reports received other than those on standard distribution; no typing or filing of catalog cards for individual reports; instant access via the terminal to report literature and its location on site. This database is truly a boon, not only to the Library staff, but to everyone on site who has occasion to use the report literature.

Other progress in automation is achieved through the Research Library's subscription to computer-assisted services offered by OCLC, Inc., a not for profit organization in Ohio. Their cataloging service will provide us with computer-produced cards, arranged in filing sequence, from 7 to 10 days after ordering via the terminal. By linking a Decwriter, which we have, to the OCLC terminal, we can produce labels required in processing for the book pocket, book card and book spine, by depressing a single key. Presently, all of these items are typed individually. This system will save time, relieve tedium, and reduce occasion for error. The monthly accession list will also be a computer product, requiring only duplication.

ENERGY CONSERVATION

Plant Engineering's Energy Management Coordination Group progressed towards its primary goal to develop energy retrofit projects that will reduce the Laboratory's consumption of electric power and fossil fuels. During fiscal year 1980, ten projects were prepared for funding in fiscal year 1982 totaling 4.8 million dollars. When implemented, these projects will save 232 billion Btu's of source energy per year with an annual dollar savings of 1.3 million dollars. The long range Laboratory goal is to reduce energy consumption in building and facilities by 20% in fiscal year 1985 compared with energy usage in fiscal year 1975.

To date the Department of Energy has funded BNL, through its in-house energy management retrofit program, 3.8 million dollars in fiscal years 77, 78, 79 and 80. When all of the funded projects are implemented, it is expected that the Laboratory will save 206 billion Btu's of source energy annually. This energy reduction represents 12.5% of the total energy used in building and facilities (excluding experimental) power in fiscal year 1975, the DOE base year.

During fiscal year 1980, the Laboratory's Energy Management Program report was updated and published. This report presents the Laboratory's accomplishments since 1973 when it first implemented its energy conservation program.

Examples of energy conservation projects presently under construction and projects completed during fiscal year 1980 are:

a) Installation of economizer on boiler No. 5 at the central steam plant.

b) Equipment modifications, new burners, controls, and boiler-burner management system at the central steam plant to permit maximum utilization of alternate liquid fuels.

c) Night setback and equipment turn-off in various buildings.

d) Equipment modifications to major refrigeration systems (e.g., steam absorption and centrifugal water chillers) to reduce energy input per ton output.

e) Adding or increasing the amount of wall and roof insulation on the wooden buildings through the site. Adding exterior foam insulation to trailers, and masonry buildings.

f) Relamping selected buildings with high efficiency, low energy usage fluorescent and high pressure sodium fixtures.

g) Solar demonstration project was completed at the Animal Quarantine building. The solar energy is used to preheat fresh air for the air conditioning system during the heating season and also to heat the building service hot water.

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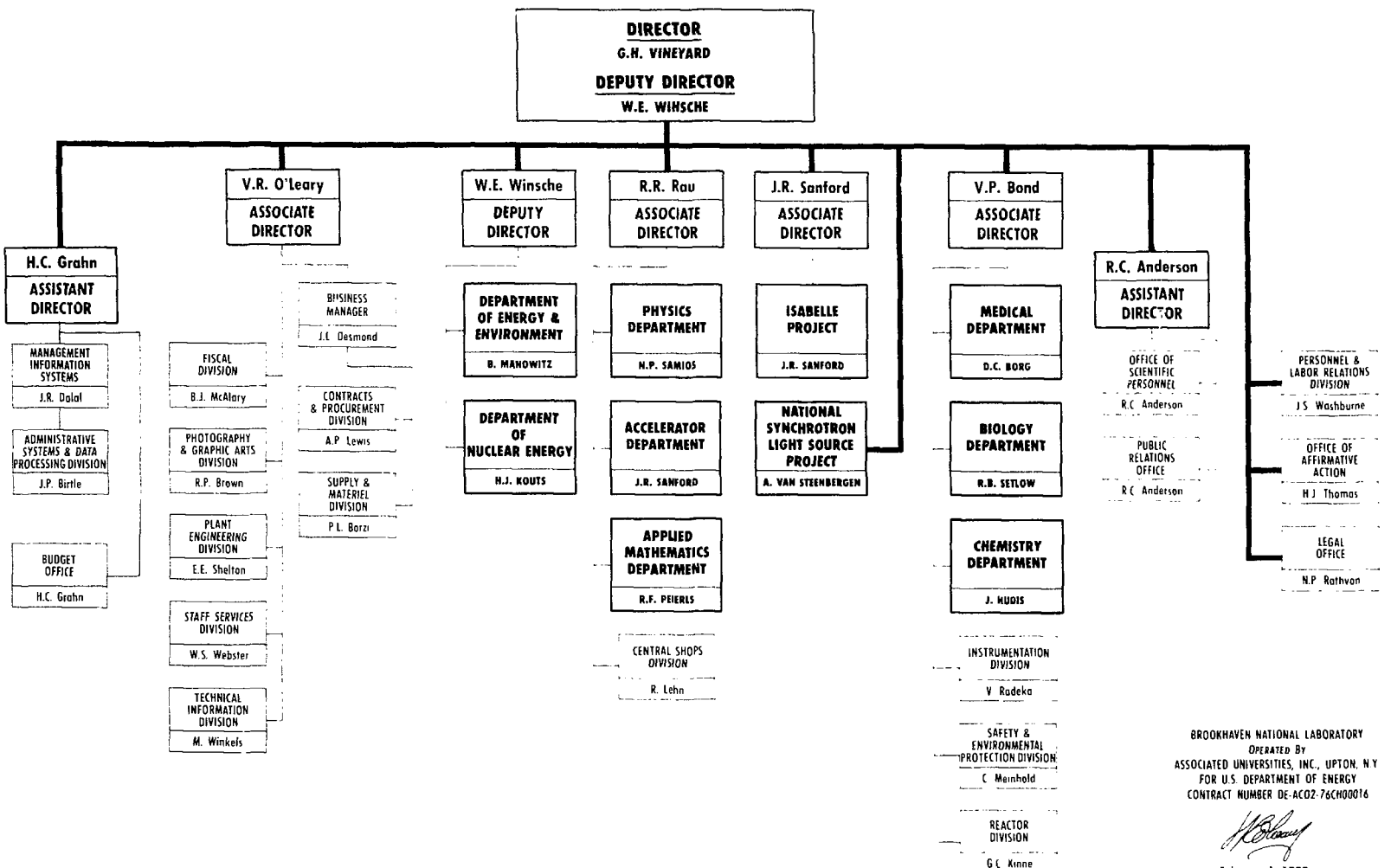
BROOKHAVEN NATIONAL LABORATORY



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