CATALOG of RESEARCH
PROJECTS
at
LAWRENCE BERKELEY LABORATORY
1985

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720
January 1985

This Catalog has been created to aid in the transfer of technology from the Lawrence Berkeley Laboratory to potential users in industry, government, universities, and the public.

For further information about this catalog, contact:

Robert J. Morris,
Office of Research and Technology Applications
50A-4112
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Telephone:
Commercial (415) 486-6502
FTS 451-6502

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

JSW

Contents

Project Descriptions by LBL Divisions

Accelerator and Fusion Research Division (AFRD)	1
Applied Science Division (ASD)	7
Biology and Medicine Division (BMD)	27
Center for Advanced Materials (CAM)	61
Chemical Biodynamics Division (CBD)	65
Computing Division (CD)	71
Earth Sciences Division (ESD)	75
Engineering and Technical Services Division (ETSD)	79
Materials and Molecular Research Division (MMRD)	85
Nuclear Science Division (NSD)	109
Physics Division (PD)	113
Name Index	115
Subject Index	119

ACCELERATOR AND FUSION RESEARCH DIVISION

K.H. Berkner, Associate Director (Acting)

(1) Plasma Heating by Various Methods
(k\$ 185)

A.N. Kaufman
R.G. Littlejohn

Our study of plasma heating embraces both basic and applied plasma theory. Basic studies include

1. Development of a unified Hamiltonian and dissipative field theory for the description of nonlinear plasma processes in complex magnetogeometry, including both resonant and nonresonant interactions.
2. Phase space techniques for the analysis of wave propagation in inhomogeneous magnetoplasmas, including tunneling and mode conversion.
3. Unification of averaging methods in diverse plasma contexts, using the mathematical theory of reduction.

Applied studies include investigations of

1. Spatial structure of drift-cyclotron-loss-cone modes and drift waves in inhomogeneous plasmas.
2. Relativistic effects in gyrokinetic theory and ponderomotive phenomena.
3. Interaction of drift Alfvén wave turbulence and ballooning modes in tokamak geometry.
4. RF stabilization of interchange modes in axisymmetric tandem mirrors.

(2) Neutral-Beam Atomic Physics
(k\$ 409)

W.B. Kunkel
R.V. Pyle
A.S. Schlachter

The purpose of our atomic physics program is to provide part of the physics input required for developing and understanding the properties of neutral-beam systems needed in the nation's magnetic fusion energy program. Such beams are used for heating and fueling mirror machines and tokamaks, and for maintaining potential barriers in mirror machines. They may also be used for current drive in tokamaks. Current activity can be classified into two areas:

1. Study of negative-ion sources that use surface and volume processes to produce the negative ions.
2. Development of diagnostic instrumentation for determining the composition, including the impurity content, of neutral beams.

As part of the first of these efforts, we are making quantitative measurements of the atomic, molecular, and surface properties relevant to negative-ion sources. We are particularly interested in the poorly understood mechanism of ion production in volume-production sources. Our aim in diagnostics development is to identify schemes capable of measuring beam composition during confinement-experiment injection. Our current emphasis is on nonperturbing laser fluorescence techniques for measuring impurity concentrations.

**(3) Neutral-Beam Development I:
Positive-Ion Base Program
(k\$ 600)**

W.B. Kunkel
R.V. Pyle
M.C. Vella

The task of the Neutral-Beam Development Positive-Ion Base Program is the timely development and demonstration of principles and techniques needed for magnetic-fusion injection systems in the 80- to 200-keV range. (Above approximately 200 keV the system efficiencies are unacceptably low for most applications.) The development of components and techniques is being carried far enough that confinement personnel can plan and design their neutral-beam injection systems with considerable confidence. Our current emphasis is on optimizing the design of our Advanced Positive Ion Source (APIS), which has been chosen as the common source module for all next-generation national program needs, and on transferring the appropriate technology to industrial vendors.

**(4) Neutral-Beam Development II:
Negative-Ion Base Program
(k\$ 2290)**

W.S. Cooper
W.B. Kunkel
R.V. Pyle

Future mirror and tokamak experiments and reactors will require efficient neutral-beam systems with injection energies of 80 keV and above. The LBL neutral-beam program includes as a major effort the development of efficient long-pulse neutral-beam systems with energies of 150 keV and higher. The present emphasis is on production and acceleration of H^- and D^- ions and on transport of the H^- and D^- beams through the radiation shielding to an efficient neutralizer.

We are pursuing two approaches to generating negative ions: production at a cesiated surface and production within the volume of a plasma. We are also developing beam transport and acceleration systems based on the concept of transverse field focusing.

**(5) Neutral-Beam Development III:
Test Stand Fabrication and Operation
(k\$ 1250)**

W.S. Cooper
R.V. Pyle

Test stands are required for developing and testing neutral-beam injection modules and system components. Our evolving test facilities serve in a sense as prototypes for neutral-beam injection systems for confinement experiments. Test stands have been and continue to be pacing items in neutral-beam development programs. At present, two facilities at LBL, test stand IIIA (150 kV, 15 A, 30 s) and test stand IIIB (120 kV, 80 A, 20 ms), routinely operate at high-power particle energies up to 120 keV.

**(6) Neutral-Beam Engineering Test Facility (NBETF) Operations
(k\$ 3000)**

W.B. Kunkel
P.A. Pincosy
R. V. Pyle

The NBETF, Phase I, is a 120-kV, 65-A, 30-s-pulse test facility having a 10% duty cycle. During 1983 it was used for general neutral-beam development of advanced positive ion sources designed at LBL and Oak Ridge National Laboratory. It is currently used for further development of the LBL source, chosen in 1984 as the common source for future program needs. The facility is operated as a national facility, scheduled by a committee with members from several national laboratories and from the DOE.

(7) High-Energy Accelerators
(k\$ 6900)

M. Cornacchia
G. Lambertson
J. Marx
C. Taylor
L. Smith

The High-Energy Accelerator R&D Group seeks to improve the design and operation of existing particle accelerators and to extend the frontiers of accelerator theory and technology as the basis for future accelerators. The group's efforts are divided into three areas: high-field superconducting magnets, beam cooling, and future facilities development.

The principal effort of the magnet group is the development of a magnet system for the planned Superconducting Super Collider (SSC). The design for a 6.5-tesla dipole magnet, produced in collaboration with Brookhaven National Laboratory (BNL), is based on the use of Nb-Ti superconductor operating at 4.5 K. We are in the process of building and testing 1-meter models of this two-in-one design; BNL will build and test longer models of our design, using our cable. We are also collaborating with industry and with academic researchers to produce superconducting cable with a higher critical current density than is now available.

The technique of stochastic beam cooling involves detecting, for single particles, deviations from the mean position and velocity of the beam, then applying corrective impulses to the same particles at a position downstream. The development, production, and testing of components for stochastic cooling of antiprotons are being carried out in support of the Tevatron proton-antiproton collider project at Fermilab. In addition, we are pursuing improvements in this technology and its more general application to feedback systems for increasing beam stability in accelerators and colliders.

Considerable effort is being directed toward conceptual design aspects of the SSC, an effort closely linked to the magnet design project. This future facilities effort can be broadly divided into three parts: basic design and parametric studies, accelerator physics and beam dynamics studies, and subsystem and component technology. During the first half of 1984, LBL also served as the host institution for the SSC Reference Designs Study, providing support of sufficient quality and depth to allow the study to complete its substantial work on schedule. During this study, AFRD physicists formed the core of the SSC Accelerator Physics Group.

(8) Two-Beam Accelerator
(k\$ 200)

A.M. Sessler
D. Prosnitz (LLNL)

We have begun an investigation of a high-gradient two-beam accelerator (TBA) with the aim of determining whether it is an attractive possibility for the next generation of linear colliders. Such an accelerator might be based on radiation generated by a free-electron laser (FEL). To explore the concept of a TBA, we have embarked on a balanced program of theoretical studies, table-top experiments with high-gradient structures, and further experimentation with the FEL at the experimental test accelerator at Livermore. We have already operated the FEL as a high-gain microwave amplifier, amplifying a 40-kW input signal to more than 100 MW.

(9) Bevalac Nuclear Physics Operation
(k\$ 18,660)

J.R. Alonso

The Accelerator and Fusion Research Division operates the SuperHILAC and the Bevalac as national research facilities for studies in heavy-ion nuclear physics, nuclear chemistry, biophysics, biomedicine, and astrophysics. The SuperHILAC has been in the U.S. vanguard for discovery of new heavy elements, in strong competition with a Soviet effort at JINR, Dubna, and more recently, a West German effort at GSI, Darmstadt. The Bevalac is unique in the opportunity it affords for the study of collisions between nuclei at energies high enough to

convert nuclear matter into hadronic matter in which protons, neutrons, excited states such as delta resonances, and free pions all coexist. In addition, a third of the Bevalac's operating time is devoted to biomedical research, including a trial program of heavy-ion cancer therapy.

The SuperHILAC, an Alvarez-type linear accelerator, provides heavy-ion beams of lithium through uranium at energies from below 1 to 8.5 MeV per nucleon. Its three injectors can supply different ion species to five different beam lines and 11 experimental areas on a time-sharing basis. In addition, a transfer line provides a beam for injection into the Bevatron, a weak-focusing positive-ion synchrotron, for further acceleration to relativistic velocities (this combined operation is called the Bevalac facility). The Bevalac can accelerate heavy ions to energies between 50 and 2000 MeV per nucleon for delivery to researchers via eight beam lines. Researchers from other laboratories and universities account for approximately half the research time at each accelerator.

Continual effort is given to improving the two accelerators—in terms of both operational efficiency and experimental facilities—so that they remain at the forefront of scientific investigation. One such effort has been the accelerator improvement project to upgrade the Bevatron's local injector to make that accelerator independent of the SuperHILAC for beams of silicon and all lighter ions. The amount of downtime required to switch beams back and forth from biomedical to nuclear research has thus been reduced, making more research time available to both programs. Accelerator improvement projects to increase ion intensities are also under way.

(10) Heavy-Ion Fusion Accelerator Research (k\$ 3745)

D. Keefe

The basic objective of this program is to assess the suitability of heavy-ion beams as igniters for inertial confinement fusion (ICF). A specific accelerator technology, the linear induction accelerator, has been studied and has reached the point at which its viability for ICF experiments can be tested.

In keeping with the national plan for heavy-ion fusion research, a two-part program will be carried out. In the first, the multiple-beam experiment, we will develop and test beam-focusing and induction accelerator modules suitable for use in the subsequent High-Temperature Experiment (HTE). This second part of the program will entail the construction of an induction linac that can heat a solid-density plasma to a temperature of 50-100 eV.

Major elements of the program are aimed at resolving four key technical issues now confronting the application of induction linac technology to ions:

1. Predicted transverse space-charge-imposed current limits.
2. Development of induction modules, pulsers, pulse-shaping systems, and multiple-beam transport arrays.
3. Preservation of the full six-dimensional phase space brightness and containment of the high-charge-density pulse during acceleration.
4. Final pulse compression, transport, and focusing of the beam on a small target.

(11) Advanced Photon Systems
(k\$ 2300)

D. Attwood
T. Elioff
R. Yourd

Recent advances in permanent-magnet insertion devices (wigglers and undulators) for electron storage rings have produced significant increases in light intensities available for research in the vacuum ultraviolet and x-ray regions of the spectrum. To make further advances possible, we are working on designs for storage rings with low-emittance, high-intensity electron beams, on a new generation of insertion devices, and on beam-line components capable of dissipating large power fluxes. To achieve the emittance and intensity we seek, we are working on ways to control instabilities; developing ultrahigh vacuum systems capable of averting problems caused by synchrotron-radiation-induced desorption processes; and developing the necessary beam-position sensors, control systems, pulsed magnet systems, and rf systems. Efforts in insertion device development include new vacuum chamber configurations, multiundulator systems for generating variably polarized light, and single-pass free-electron lasers for the UV and x-ray regions of the spectrum.

(12) Center for X-Ray Optics
(k\$ 1400)

D. Attwood

Rapid progress in the development of intense sources of radiation in the vacuum ultraviolet and soft x-ray regions of the electromagnetic spectrum has created a need for new optical components and techniques for users of this radiation. The Center for X-Ray Optics, created in 1983, has as its charter the development of technologies required for the utilization of emerging sources of XUV radiation in science and industry. The Center has already organized laboratories and collaborations that will lead to new technologies for the efficient transport, focusing, dispersion, and detection of radiation with proton energies from 20 eV to many keV. The activities of the Center have the common goal of extending the use of XUV radiation for basic and applied research.

(13) Studies in Nonlinear Dynamics
(k\$ 100)

A.N. Kaufman
R.G. Littlejohn

Our theoretical studies of nonlinear dynamics are oriented primarily toward an understanding of processes in continuous media, such as waves, fluids, and plasmas. A unifying concept is the use of modern differential geometric methods. Major components of the program are

1. Phase space and complex manifold techniques for multidimensional wave propagation in inhomogeneous and anisotropic media.
2. Unification of averaging methods in diverse physical contexts, making use of the mathematical theory of reduction.
3. Analysis of continuous Hamiltonian dissipative systems, with a view to studying equilibrium, stability, and transport.

(14) Free-Electron Laser at the ETA
(k\$ 360)

A.M. Sessler
D. Prosnitz (LLNL)

The free-electron laser (FEL) at Livermore's experimental test accelerator (ETA) is being used for basic studies of FEL physics. One of the aims of these studies is an accurate assessment of whether such a system might be used for electron-cyclotron resonance heating of plasmas. Ongoing studies include measurements of output microwave power as a function of input power, wiggler parameters, and beam parameters (including current, emittance, and energy). We are also measuring electron beam characteristics (such as energy loss and energy spread) in our efforts to optimize FEL performance.

APPLIED SCIENCE DIVISION

E.J. Cairns, Associate Director

- (1) **Management of the Technology Base Research (TBR) Project for Electrochemical Energy Storage**
(k\$ 4358)

E.J. Cairns

LBL is the lead center for management of the TBR Project, which is supported by DOE's Office of Energy Systems Research, Energy Storage Division. The purpose of this project is to provide the research base that supports DOE efforts to develop electrochemical technology for electric vehicle and stationary energy-storage applications.

The general objective of the TBR project is to help provide advanced electrochemical systems that can satisfy stringent performance and economic requirements for electric vehicle and stationary energy-storage applications. The specific goal of the project is to identify the most promising electrochemical technologies and transfer them to industry and/or another DOE program for further development and scale-up.

General problem areas addressed by the project include identification of new electrochemical couples for advanced batteries, determination of technical feasibility of the new couples, improvement of battery components and materials, establishment of engineering principles applicable to electrochemical energy storage and conversion, and assessment of fuel-cell technology for transportation applications. *Major emphasis is given to applied research that will lead to superior performance and lower life-cycle costs.*

- (2) **Process Development Studies on the Bioconversion of Cellulose and Production of Ethanol**
(k\$ 200)

H. Blanch
C. Wilke

Biomass represents a large renewable resource that may be viewed as a form of stored energy. The conversion of biomass to its component sugars and their subsequent fermentation to produce ethanol are the prime objectives of this work. Biomass is available in the form of whole trees, grains, and agricultural residues. The project investigates both enzymatic and acidic hydrolyses of biomass to hexose and pentose sugars. Basic information on the kinetics of these processes is to be obtained. This information can then be used to develop low-cost processing schemes for sugar production. High-productivity fermentations to convert these sugars to ethanol or other chemical feedstocks are to be developed. Fundamental studies on metabolism in high-cell-density cultures will be made. This will be combined with basic studies on ethanol separation from the fermentation broth, using novel, low-energy schemes. *With this basic data, overall process evaluation can be undertaken.*

- (3) **Metal Coordination Chemistry**
(k\$ 170)

R. Fish

This program will develop an alternative approach for the removal and recovery of metal compounds from heavy oils by complexing the various inorganic and organometallic compounds present in the oil with multidentate ligands that potentially can be attached to a polymeric backbone.

These studies include speciation, or molecular characterization, of those metal compounds of vanadium, arsenic, and iron known to be in the heavy crude and shale oils. The speciation studies are being carried out by a new technique that combines a high-performance liquid chromatograph (HPLC) with a graphite-furnace atomic absorption spectrometer (GFAA) and

that allows a rational approach to the applicable coordination chemistry for these metal compounds.

The goal of the coordination chemistry studies is to create complexes of the speciated inorganic and organometallic compounds with new multidentate ligands that can be attached to a polymeric backbone for use in percolation-type sorption columns. The structures of both the indigenous and the synthesized model complexes are being determined by various spectroscopic techniques such as nuclear magnetic resonance spectroscopy, mass spectrometry, ultraviolet spectroscopy, and single-crystal x-ray crystallography.

(4) Breakup of Liquid Filaments
(k\$ 28)

M.M. Denn

The breakup of liquid filaments and sheets is a fundamental problem of interest in many areas of technology, including the manufacture of synthetic polymer and glass fibers and aerial dissemination. Existing theories of breakup appear to work for low-molecular-weight liquids, but they are unsuccessful when polymer additives are included. The reason here appears to be that the time scale of initial disturbance growth dominates the combined growth and breakup process for low-molecular-weight materials, but nonlinearities associated with the presence of the polymer delay the latter part of the growth process sufficiently to allow the breakup time scale to dominate. The presence of the polymer additive may cause substantial alteration of the stress field in the region of breakup, and this may also affect the time for ultimate filament rupture. The work focuses on the mechanics of a thin sheet or filament that is being elongated, to determine the processes leading to filament rupture and to develop predictive capabilities regarding rupture.

(5) Advanced Thermal Energy Storage Technologies
(k\$ 300)

E.J. Cairns

The Advanced Thermal Energy Storage Technologies Program comprises four research projects: (1) The Solid State Radiative Heat Pump, (2) Thermochemical Conversion and Storage Using Small Particles as Heat Exchanger and Catalyst, (3) Three-Phase Thermal-Energy Storage Module with Constant or Variable Thermal Conductance, and (4) Gas-Loaded Heat Pipes for Enhanced Conductance and Integrated Thermal-Energy Storage Control. Projects are selected because of their potential to lead to thermal-energy storage systems with high second law efficiencies as well as the potential for meeting projected cost and energy-capacity criteria for commercialization.

(6) Battery Electrode Studies
(k\$ 300)

E.J. Cairns

The objective of this research is to study the behavior of electrodes used in secondary batteries and to investigate practical means for improving their performance and lifetime. Systems of current interest include ambient-temperature rechargeable cells with zinc electrodes, rechargeable high-temperature cells, fuel cells, and photoelectrochemical cells. The approach used in this investigation is to study life- and performance-limiting phenomena under realistic cell operating conditions.

(7) Separations by Chemical Complexation
(k\$25)

C.J. King

This project explores the use of separation processes based upon reversible chemical complexation for purposes of recovering polar-organic substances from dilute aqueous solutions. Solutes of interest include alcohols, glycols, carboxylic acids, and amines. Specific examples include ethanol, butanol, acetic acid, and amino acids, which together already consume a substantial amount of the national energy for recovery. Methods of approach include characterization of bonding parameters for complexation, along with factors influencing regeneration of the separating agent, and other critical process parameters.

(8) Condensate Wastewater
(k\$ 110)

C. J. King

This project deals with physicochemical processing of condensate waters from gasification and liquefaction of coal, with the goal of making them suitable for recycle as cooling-tower make-up water. Processing methods principally considered are solvent extraction, stripping, evaporation, and adsorption, as well as combinations of these. Of particular interest are new processing approaches that will allow removal of Chemical Oxygen Demand (COD) and removal and recovery of ammonia in ways not now possible and/or that will substantially reduce the costs of processing. Improved analytical techniques are being developed as needed.

(9) Passive Research and Development
(k\$ 1360)

R. C. Kammerud
M. R. Martin
J. W. Place

The passive program at LBL is directed at theoretical and experimental investigations of the thermal performance implications of passive design strategies; emphasis is given to passive and hybrid cooling of commercial buildings. In this context, the objectives of the program are:

1. Develop analytic descriptions of the thermal processes that occur within a building or between a building and the environment. These heat-transfer algorithms are based on empirical data and/or analysis from first principles.
2. Evaluate the effectiveness of passive systems in reducing the heating, cooling, and lighting energy consumption in the United States and identify effective criteria for passive system design optimization.

Heat-transfer research projects are: (1) examining natural convection within buildings and between buildings and the environment and (2) calculating the thermal performance of ventilation cooling in nonresidential buildings. Passive systems evaluation activities are directed at characterizing the impacts on building performance of specific passive strategies using building energy analysis techniques. This includes examination of the relationships between heating, cooling, and illumination energy consumption and climate parameters, building structure, building use patterns, Heating, Ventilation, and Air Conditioning (HVAC) system, and the local utility. Specific passive techniques that are under evaluation are: direct-gain space heating, daylighting, solar load control, ventilation, cooling, and thermal mass.

(10) Active Solar Cooling
(k\$ 792)

M. Wahlig

This project includes research on advanced absorption cycles for solar cooling, systems analysis to determine future research requirements for the active solar cooling program, and technical support activities to assist DOE and DOE contractors in the advancement of solar cooling technology.

Advanced Chiller Research. LBL is conducting in-house research on advanced thermodynamic cycles for solar cooling. The resulting advances in absorption-cycle cooling technology are expected to lead to higher-efficiency solar-absorption cooling systems capable of displacing the use of conventional electric-driven air conditioners. The research work consists of conceptual analysis and detailed design of advanced absorption cycles, followed by laboratory experiments to prove the validity of these new high-efficiency cycles.

Systems Analysis. LBL has a major research effort in systems simulation and economic analysis for active solar space-conditioning technologies, including: refinement, use, and documentation of methodologies for determining the future research requirements; detailed analysis of the sensitivity of performance and economics to critical design factors; and determination of the impact of controls on the performance of absorption and Rankine cooling systems.

Technical Support. This is in the form of program planning, technical monitoring of projects, and related tasks will be provided for DOE-supported research activities in solar-absorption and Rankine-cycle cooling.

(11) Optical Glazing Materials
(k\$ 660)

S. Selkowitz
A. Hunt

We are identifying and investigating fundamental physical processes, materials, and devices having a high potential for increasing the energy efficiency of glazed apertures in buildings. Four broad, functional categories are being studied: (1) low conductance, high transmittance glazings—systems that minimize conducted and convected heat transfer while maximizing radiant transmission; (2) optical switching materials—materials whose optical properties can be altered in response to environmental conditions; (3) selective transmittance glazings—glazings with angle-selective properties or spectrally selective properties to control solar gain; and (4) daylight enhancement—systems to collect, transmit, and distribute daylight within buildings. In each area we examine the potential of appropriate optical technologies such as interference coatings, microstructured surfaces scattering media, optically active materials, holography, guided wave optics, etc., as well as thermal control techniques.

The work includes performance predictions for novel systems to identify potential savings, a review of each optical technology, and an experimental program to investigate the most promising technologies. The work will also result in a multiyear research plan to guide LBL as well as other DOE contractors. Program staff would provide scientific oversight and review of all DOE-supported efforts in this program area.

(12) Direct Radiant Heating of Particle Suspensions
(k\$ 225)

A. Hunt

The purpose of this project is to investigate the direct solar radiant heating of particle suspensions. This work is being undertaken to develop a technology base for a new class of unique, direct-absorption solar receivers. These receivers use concentrated sunlight to drive chemical reactions in gas-particle mixtures to produce useful fuels and chemicals. The successful design of direct-absorption receivers requires an understanding of the properties of particle suspensions as they are heated by concentrated sunlight. The goals of this program are to obtain fundamental data, perform calculations, and carry out experimental investigations regarding the optical, thermodynamic, and chemical processes involved in the solar heating of particle suspensions. Once sufficient data are obtained, a realistic evaluation will be made of the possibilities and constraints in the design of direct-absorption receivers for the production of fuels and chemicals from concentrated sunlight.

(13) Sol-Gel Processing
(k\$ 30)

A. Hunt

This project is investigating the technique of sol-gel processing for the production of high-temperature ceramics, with the goal of developing an alternative preparation process. Traditional ceramics manufacture relies on the production of small particles of pure or mixed compounds that are sintered at high temperature to form a cohesive mass. These materials are composed of particles with sizes from approximately one micron to hundreds of microns. The resulting granular composition is responsible for the mechanical properties.

The sol-gel process for manufacturing materials is a way of producing very fine-grained solids that possess structures in the size range of 0.005 to 0.01 microns. The resulting material has superior properties to traditional ceramics because of the extremely small structures. It also is a means of producing materials with mixed compositions by combining the colloidal sols in the early stages of preparation. The technique consists of producing a colloidal solution of the desired composition, allowing it to gel, and then removing the liquid trapped in the interstices. The material may be molded to arbitrary shapes and does not require high-temperature processing. The project will survey sol-gel processing for ceramic materials and prepare a plan for an experimental and analytical effort to develop this technique into an alternative ceramic preparation technique.

(14) Microparticles as an Advanced Media for Heat Exchange and Catalysts
(k\$ 75)

A. Hunt

The purpose of the research is to investigate potential thermochemical storage reactions of gases at the surface of suspended particles in the presence of sunlight. Small particles can absorb radiant energy and act as catalytic sites for endothermic reactions. The reaction products are separated, cooled, and stored at ambient temperature. The stored energy is released by combining the reaction components under suitable circumstances to produce process heat or to drive a turbine.

Many reversible reactions for heat storage require high temperatures to initiate. Direct radiant heating insures that the highest temperatures occur directly at the reaction sites. The particles may be separated, reacted, or vaporized to stop the back reaction. Photolytic-induced catalysis at the sites of the small particles may significantly enhance the reaction rates over those derived from purely thermal effects. The approach will be to identify potential reactions, assess their suitability for storage applications, and perform experimental studies of the processes.

(15) Photochemical Conversion of Solar Energy
(k\$ 117)

L. Packer

This program seeks to characterize the molecular events associated with the photochemical conversion mechanisms in bacteriorhodopsin: this light- and temperature-stable protein, which operates via a photocycle to develop a proton current, contains retinal as a chromophore and is the only protein found in the purple membrane isolated from halobacteria.

Approach. Bacteriorhodopsin is investigated in the natural membrane and in reconstituted artificial membranes. Chemical modification with a wide variety of group-specific reagents is used to identify those amino acids that are essential for the photocycling activity and the simultaneous proton pumping through the molecule. These studies are aided by the investigation of isotope effects and by the use of laser-flash photolysis measurements and electron spin resonance (ESR) spin-probe and labeling techniques, which correlate individual steps in the photocycle with electrochemical and structural events within and across the protein. Analogous

studies are being undertaken on a recently discovered retinal-lacking protein (mutant R_mW), which can be reconstituted into a similar light-activated proton pump by the addition of retinal and retinal analogues. The anticipated benefits of this program include understanding of the molecular basis of the photochemical energy conversion by retinal proteins and their use for development of photovoltaic cells.

(16) Energy Efficient Buildings Studies
(k\$ 4304)

A. H. Rosenfeld

Approximately 38% of the energy consumed annually in the U. S. is used in buildings. The Energy Efficient Buildings Program of LBL investigates ways of reducing this consumption through research in the following areas:

The Energy Performance of Buildings Group investigates ways of increasing energy efficiency by tightening building structures and reducing thermal losses. This project (1) assesses thermal performance of building envelope systems, (2) assesses infiltration sources in buildings, (3) disseminates research findings and maintains exchange programs for scientists and technical experts, (4) develops residential energy audits [the Computerized Instrumented Residential Audit (CIRA)], and (5) develops low-cost instruments for monitoring whole-building performance [the Energy Signature Monitor (ESM)]. (M. Sherman)

The Ventilation and Indoor Air Quality Group furnishes a scientific basis for determining energy-efficient ventilation standards and systems that provide for the health and comfort of occupants. This group also seeks to characterize indoor air pollutants and develop comprehensive indoor air quality recommendations. This project (1) reviews and assesses ventilation requirements and indoor air quality, (2) reviews and assesses mechanical ventilation systems, (3) investigates policy issues, and (4) disseminates information. (D. Grimsrud, A. Nero)

The Building Energy Simulation Group continues to improve its DOE-2 computer model for predicting energy use in buildings and for assisting architects, engineers, and others in the private and public sectors. This project (1) oversees the maintenance and documentation of the DOE-2.1 computer program for the energy-use analysis of buildings, (2) designs and implements an advanced research building energy-use and performance model, and (3) tests and validates the DOE-2 program to ensure that current and new algorithms accurately predict energy performance of buildings. (J. Hirsch)

The Windows and Daylighting Group develops the technical basis for determining optimal fenestration (window and skylight) performance to minimize heating and cooling loads in buildings and conducts research on using daylight to reduce energy consumption and peak demand. The group's work encompasses the following areas:

1. Analytical and experimental modeling, aimed at developing and validating a range of computer models and experimental techniques for determining the energy-related performance of fenestration materials, components, and systems; accounts for daylighting effects and thermal performance.
2. Materials science studies, aimed at developing the analytical models and experimental techniques for characterizing the performance of advanced optical materials as applied to fenestration.
3. Fenestration optimization, which uses simulation studies to generate the technical performance data required for developing a comprehensive and usable set of guidelines for optimizing the energy-related performance of fenestration as a function of building type, occupancy, and climate.

4. *In-situ* testing, which has the goal of developing a data base on fenestration performance based on carrying out experimental studies in occupied buildings and in controlled field test facilities; these data will be used to validate computer models of component performance and optimal design strategies. (S. Selkowitz)

The Buildings Energy Data Group compiles, evaluates, and publishes measured energy performance data for low-energy buildings. Empirical data are compared with performance predictions and used to update estimates of regional technical potentials for conservation. The tasks of this project are to (1) collect and critically review evaluations of new and existing homes, commercial buildings, and energy-efficient appliances and equipment and (2) collaborate with utilities and other nonfederal organizations in establishing and updating a public-domain data base on technologies for improving energy efficiency in buildings. (J. Harris)

(17) Indoor Air Pollution

A. V. Nero

(k\$ 288)

This project is directed at characterizing indoor air pollution and assessing the health and exposure implications of indoor pollutant sources and of residential energy-conservation programs that would reduce ventilation in buildings and thereby contribute to a build-up of indoor pollutants, e.g., CO, NO₂, respirable particles, radon, radon daughters, and organic compounds such as formaldehyde. These substances can be generated by combustion appliances or emitted from building materials, ground soil, or furnishings. This project seeks (1) to characterize indoor pollution; (2) to determine the important sources, abundances, and emission rates of indoor air pollutants in buildings; (3) to assess schemes for controlling indoor air pollutants; (4) to study the health risks from indoor air pollution; and (5) to assess the impact of various energy-conservation strategies on indoor air quality. The study initially focuses on the characterization of combustion-generated indoor air pollutants and on a risk assessment of radon and other major indoor air pollutants. This assessment will consider the current risk from indoor air pollutants as well as the potential added risk associated with specific energy-conservation strategies.

(18) Radon Characterization

A. V. Nero

(k\$ 150)

The purpose of this study is to characterize the sources and concentrations of indoor radon and its radioactive decay daughters. The objectives are to determine the range and frequency of the daughter concentrations to which humans are exposed indoors; to assess the impact on these concentrations of programs that would reduce energy requirements in buildings; and to analyze the effects of strategies to control exposures to radon daughters. Indoor radon may originate in the soil or rocks that underlie buildings, in building materials, and in domestic water supplies. Energy-conservation measures, particularly reduced ventilation, may increase indoor concentrations of radon and its daughters, thus increasing the radiation to which occupants are exposed. The project (1) performs laboratory measurements of the radioactive content and radon-emanation rates of building materials (e.g., concrete, gypsum, and solar rock beds) and of the soil and rock underlying buildings; (2) conducts laboratory and research-house measurements of radon and radon daughters and studies removal processes; (3) performs field measurements of sources and concentrations to complement laboratory work; (4) using physical models, evaluates typical exposure levels, techniques to be used in large-scale surveys, and specific control procedures; and (5) conducts laboratory and field measurements to characterize the transport processes by which radon enters buildings.

**(19) Bonneville Power Administration
(BPA) Technical Support
(k\$ 200)**

J. Harris
A. Meier

In recent years, demand for electricity in the Pacific Northwest has grown to equal nearly all the hydroelectric generating capacity available in the region. Although the cost of generating this electricity is quite low, the projected cost of electricity from new capacity is so high that, in many instances, it is more economical to curb demand through conservation. In 1980, the United States Congress ordered BPA, supplier of much of the electricity in the Pacific Northwest, to rely as extensively as possible on cost-effective conservation and renewable resources in responding to growing demands for electricity, while at the same time protecting the environment. These two events have made it important to BPA that buildings use energy more efficiently in the future. Because the Energy Efficient Buildings Program and LBL have a national reputation for energy research, BPA has asked the program for technical support. The current project involves compiling and analyzing measured energy-performance data from new commercial buildings in the BPA service area. This compilation, which is a subset of the existing commercial-building compilation, will focus on new, energy-efficient buildings. LBL will identify which buildings are energy efficient and correlate their performance to technical features.

**(20) Lighting Technology
(k\$ 2085)**

S. Berman

Lighting systems in buildings account for 6% of national energy consumption. LBL is carrying out a comprehensive program aimed at bringing about substantial energy savings in this area by (1) supporting long-term and high-risk research into new energy-efficient lighting systems and (2) carrying out investigations that provide the community of lighting users with information on the impact of advanced lighting technologies on man, machinery, and the environment.

The program supports research and development leading to the effective and efficient employment of illumination. This includes long-term efforts to develop more efficient light sources as well as to provide the means of on-site control of those light sources. In addition, a series of fundamental experiments is being conducted to relate illumination, visibility, health, and environment to productivity to assess effective lighting strategies.

**(21) Advanced Lighting Design
(k\$ 96)**

S. Berman

This work consists of two projects. One project is the characterization of solid-state ballast and auxiliary control equipment for operating standard F40 T-12 fluorescent lamps. The input and output characteristics have been measured for nine types of solid-state ballasts and twelve types of lighting control systems. The work shows large variance in the performance of the equipment.

The second project is to determine the optimum position for a photocell for sensing the ambient natural lighting. The object is to provide a constant illumination level supplied by electrical and natural light. The study required constructing a model room (one-third size) as the vehicle to collect the data. The room has fenestration and can be rotated 360° such that data from all major directions can be obtained. The model is located on the roof of one of LBL's buildings.

(22) Field Measurements of Daylighted Buildings
(k\$ 95)

S. Selkowitz

A field monitoring program is being conducted to measure the overall energy performance of a five-story, 400,000-ft² office building in Sunnyvale, California. The performance of specific components and subsystems (e.g., daylighting features and automatic electric-light dimming controls) is also being measured. This office building represents the state of the art in energy-efficient design, including innovative daylighting design features and a low-energy air distribution system. Data collection and analysis over several years will allow us to determine the effects of daylighting strategies on load profiles and peak loads and the impact of glazing systems on daylighting savings and cooling costs. Results will also provide feedback on LBL's sky simulator, which was used to test the building design, and the DOE-2 energy analysis program, which was used to predict energy consumption in the building.

(23) Daylighting Technology Assessment
(k\$ 50)

S. Selkowitz

This project provided for a state-of-the-art assessment of daylighting technologies and a determination of the potential energy and load management savings achievable in commercial buildings (in New York State). Recommendations for new research needs were developed. Project tasks included an assessment of technical performance issues (daylight availability, thermal control, glare control, lighting control, and load management).

(24) Surface Microstructure for Advanced Glazing
(k\$ 25)

S. Selkowitz

A significant fraction of the energy used for space heating, cooling, and lighting can be saved by using advanced window coatings to control radiant energy flows into and out of buildings. The optical performance of most coatings depends primarily on the materials properties, which are in turn influenced by deposition conditions (e.g., pressure, electric field, etc.). An alternative approach is to use the geometry and structure of the applied coating (as well as the properties of materials) to determine ultimate glazing performance. Potential applications include: low-emittance coatings, anti-reflective coatings, concentrators for beamed daylight systems, and angular transmission control. We will explore the feasibility of several of these.

(25) Naval Lighting Project
(k\$ 61)

S. Berman

A core ballast system has been submitted that has an improved power factor (PF) and meets the harmonic specifications. Currently the PF is about 60% with a 7% third harmonic. The new design has a PF of 90% and a third harmonic of 2%, which meets the Navy's 3% maximum specifications. Twenty of these ballasts will be purchased and submitted to LBL for evaluation. This includes testing the overall electrical performance, efficiency, lumen flux output, and reliability. The improved power factor will have a major impact on the sizes of wire required for illuminating ships by reducing the electrical power that must be supplied.

(26) Field Surveys of Indoor Air Quality in the Pacific Northwest
(k\$ 800)

D. Grimsrud

The Pacific Northwest Electric Power Planning and Conservation Act (Regional Act) authorized the Bonneville Power Administration (BPA) to undertake cost-effective conservation programs to help meet the Administration's load obligations. One of BPA's proposed methods to meet these objectives involves a regionwide house-tightening program that includes caulking, weatherstripping, and installing outlet and switch box gaskets and storm

windows. Although house tightening effectively achieves its purpose of reducing infiltration, it also may result in an increase in the concentration of air pollutants, particularly those generated by indoor sources.

This study is designed to examine the effect of weatherization on indoor air quality in residential buildings in the Pacific Northwest. The project is divided into three major areas:

1. Measurement of the distribution of pollutant concentrations in existing housing.
2. Examination of the effects of weatherization measures that reduce air leakage on pollutant concentrations.
3. Field testing of various indoor air quality control strategies in houses where high levels of pollutant concentrations are found.

The project will extend through June 1986.

(27) Concentrations of Indoor Pollutants Data Base
(k\$ 150)

D. Grimsrud

Exposure to pollutant concentrations in buildings is emerging as a major component of a population's total exposure to air pollutants. As this is recognized, the need for more information about indoor air quality increases. This need is being met by research and field measurement and by collection and organization of existing measured data.

This project is designed to gather published and unpublished research results and organize them into a data base that is openly accessible to a wide audience of researchers, policy makers, and others interested in the issue of indoor air quality. An accessible source of measured data will serve agencies and trade organizations engaged in providing guidelines and state and local government agencies responsible for establishing building and ventilation standards.

(28) Personal Exposure to Methylene Chloride
(k\$ 90)

D. Grimsrud
A.V. Nero

This study shall characterize personal exposure to airborne methylene chloride (CH_2Cl_2) from consumer products, examining a model-use pattern in an environmental chamber. More than 0.5 million pounds of CH_2Cl_2 are produced annually in the U.S., primarily for use in paint strippers and aerosol paints. CH_2Cl_2 that is retained on inhalation is metabolized to CO, leading to anoxic stress from elevated levels of carboxyhemoglobin; in addition, a study has associated salivary-gland carcinoma with CH_2Cl_2 inhalation. We shall examine exposures to paint strippers and aerosol paints as important examples of exposures to such airborne organics from consumer products used indoors. The immediate result of this work will be quantitative exposure data for these particular products, which can be used as a basis for assessing associated health risks, to the extent that dose-response information is available. Experiments shall be conducted in LBL's new room-sized environmental chamber using a range of air exchange rates. Both area and breathing-zone concentrations shall be measured during and (for the area measurements) after use. These shall be compared and examined within the context of a predictive model for describing concentrations of airborne organics in residential indoor air.

(29) Pollutant Emissions and New Heater Designs
(k\$ 85)

D. Grimsrud
A.V. Nero

This study shall determine the potential contribution of unvented heaters to pollutant levels in the home. New heater designs are now entering the market in response to previous work conducted at LBL and elsewhere that showed excessive generation of combustion pollutants by these sources. This study will examine the emissions from these sources in both normal and maladjusted operating conditions. The results will be used as inputs into a future modeling effort that will be undertaken at LBL to predict population exposure to pollutants from these sources.

(30) Radon Source Characterization
(k\$ 120)

A.V. Nero

This work will review our current state of understanding of the sources of indoor radon in U.S. homes and will extend it in two substantial ways. (1) It will examine the information available on the factors affecting radon generation or transport and develop a generic approach for using this information for assessing the potential radon source strength of geographic areas under consideration. The factors to be considered are radionuclide content of source materials, the geologic nature of the area, and the permeability of local materials, as well as the building-related and meteorological factors that affect radon entry. (2) It will also examine the information currently available on radon in domestic water supplies and on the emanation of radon from water when used, as a basis for constituting a predictive capability for assessing the effect of water-borne radon on indoor exposures to radon daughters. Experimental work will be carried out, as necessary, to provide a basis for this predictive capability.

(31) Source Characterization of Combustion Appliances
(k\$ 100)

D. Grimsrud

Source strengths of combustion appliances have been measured using two distinct procedures. In the chamber technique, developed at LBL, pollutant concentrations are measured in a single-zone, well-mixed chamber containing the pollutant source. Combustion air for the device contains pollutants emitted; in particular, the effect of oxygen depletion in the chamber on the combustion process can be determined directly.

An alternate procedure commonly used by the gas industry is a hood technique that is an American National Standards Institute standard. This test, originally designed to measure CO emissions from gas appliances, has been extended to be used with other pollutants. A hood above the combustion device captures combustion products, and the concentration of a particular pollutant is compared to the concentration of carbon dioxide to determine the emission rate.

This study will develop a measurement protocol that can be used to compare the hood and chamber studies; compare the results from standard unvented space heaters using the two procedures; and use these results to develop a field procedure to measure source strengths of combustion devices for survey applications.

(32) Coal-Slurry Diesel Engines
(k\$ 200)

F. Robben

Supporting work aimed at assessing the coal-slurry diesel-engine will be carried out. Such engines, if technically feasible, will have significantly higher efficiency than steam turbines, the traditional coal-burning engine. Both the combustion and wear problems appear capable of solution, based largely on extensive development efforts carried out in Germany during the period 1930-1944. Medium-speed coal-water slurry diesel engines would efficiently replace a

significant fraction of fuel oil in this country. The ignition and combustion of coal-water slurry fuels under diesel conditions are being experimentally determined in a special single-cycle engine with transparent cylinder walls. High-speed cinephotography is the principal diagnostic method to determine coal-water slurry fuel-ignition and combustion characteristics. The dependence of the combustion parameters on the fuel properties and engine conditions will be explored. Various methods of enhancing the combustion rate will be considered. The projected operating characteristics of coal-slurry diesel engines of different sizes and configurations will be assessed. The potential market for such engines and the associated economic and energy benefits will be considered. This work will be coordinated with the effort at the Morgantown Energy Technology Center to assess and plan for the development of such engines and with work at other laboratories related to coal-slurry diesel engines.

(33) Lean Engine Combustion
(k\$ 200)

R. Sawyer

Premixed lean combustion provides a promising means for improving efficiency, extending fuel tolerance, and reducing emissions of automotive engines. Two unique square-piston, compression-expansion machines that provide full optical access to the combustion process under conditions simulating those of reciprocating engines have been designed, constructed, and demonstrated. These are used for the study of ignition processes, flame structure and propagation, wall heat-transfer processes, and flow-field studies.

In addition to the two engine simulators, two constant-volume cells are also being used to study ignition processes and flame-heat transfer interactions. Theoretical models for the processes observed are being developed to aid in the interpretation of experimental data and to provide components for larger-engine combustion modeling efforts.

(34) Combustion of Kerosene Heaters
(k\$ 110)

N.J. Brown

This research has as its primary objective the modification of the combustion process to optimize the conservation of energy. Emphasis is placed on acquiring an understanding of the combustion process involved with kerosene burning on a wick, with the purpose of achieving energy conservation through control over combustion. There are two strategies for enhancing the conservation of energy with respect to the use of unvented combustion sources. The first of these is concerned with increasing the efficiency of combustion by increasing the extent of combustion. Specifically, the concentrations of CO, hydrocarbons, and particulates that have been reported in the literature as emissions from unvented kerosene heaters are indications of incomplete combustion during start-up and steady-state operation. We are elucidating the experimental parameters that affect the completeness of combustion. The second strategy for conserving energy is to reduce the need for ventilation by reducing the emission of noxious compounds.

(35) Aerosol Chemistry
(k\$ 256)

T. Novakov

The goals of this project are (1) to study the chemical kinetics and mechanisms of heterogeneous atmospheric reactions and to assess the contribution of these processes to the overall air pollution, (2) to assess the contribution of primary particulate emissions to the total aerosol burden, and (3) to establish the relative roles of photochemical and nonphotochemical aerosol-producing reactions. The emphasis of the chemical reaction studies is on the formation of sulfate, nitrate and other nitrogenous species, and organic aerosol material. Of special interest are heterogeneous reactions that take place in liquid water droplets catalyzed by primary particulates such as soot and trace metals.

(36) Turbulent Combustion
(k\$ 254)

F. Robben

Combustion takes place in the turbulent mode in almost all practical combustion systems, and a proper understanding and modeling of the interaction between fluid mechanical turbulence and combustion heat release are necessary for the rational design of advanced-performance combustion systems. The objective of the present research is to develop an experimental data base for premixed turbulent combustion that will give insight into techniques and approximations suitable for numerical modeling and that can be used for quantitative comparison with numerical modeling calculations. At present, two experimental systems are being studied using laser-based diagnostics (laser Doppler velocimetry and Rayleigh scattering): lean combustion supported in a turbulent heated-wall boundary layer and flame propagation in grid-induced turbulence. The heated-wall boundary layer results indicate that, at low Reynolds number, combustion-heat release reduces the turbulent kinetic energy. With grid-induced turbulence, a stabilized flame increases the upstream (unburned) turbulent kinetic energy slightly while reducing the turbulence in the burned, post-flame region. More advanced diagnostics to measure cross correlations between fluctuation measurements are being developed and will be used to obtain some parameters important for using the density weighted (Favre) averaging modeling approximation.

(37) Novel Photothermal Spectroscopic Techniques for the Characterization of Surfaces and Thin Films
(k\$ 70)

N. Amer

During the past few years we have employed the concept of optical heating for the ultrasensitive determination of optical absorption (e.g., the detection of one part per trillion of gaseous pollutants). This was accomplished photoacoustically or by means of beam-deflection techniques.

We propose to extend the scope of our detection schemes by exploiting the deformation of a solid sample by optical heating. This will be done using, for example, interferometry.

The successful development of this technique will have a direct bearing on our research on amorphous photovoltaic films and on semiconductor gas sensors.

(38) Flame Radiation
(k\$ 38)

C. Tien

This project will continue the research program on flame radiation that has been conducted at the University of California at Berkeley and the Lawrence Berkeley Laboratory during the past few years. A major reorientation in research has been initiated during the past year to study infrared radiation of gases evolved from burning condensed fuels. Specific emphasis is placed on (1) infrared radiation properties of the evolved gases and (2) radiative energy absorption from a thin, nonisothermal layer of these gases. Progress has been made in the design and construction of apparatus for measuring infrared radiation of these evolved gases as well as in analytical modeling of complex spectroscopic structures.

(39) Environmental Effects/Controls—Oil Shale
(k\$ 400)

J.F. Thomas
C.G. Daughton

Oil shale developers propose that retorted (spent) shale will be disposed together with the retort process wastewaters. This "codisposal" process would serve in disposal of wastewaters while also cooling the hot spent shale, controlling dust, and moistening the shale to promote compaction. The environmental fate of compounds contained in these wastes is governed by several transport and transformation processes. This project investigates a major transport

process (volatilization) and two key transformation processes (photolysis and biodegradation). The major objectives of this research are to: (1) establish the importance of volatilization and identify and quantify the volatile organic compounds; (2) determine the impact of vapor-phase and surface-phase photolysis on the volatile/nonvolatile components; (3) determine the effect of biotransformations on volatilization; and (4) develop analytical methods for colligative water-quality parameters (especially organic nitrogen), capillary gas-chromatographic head-space analysis, and air sampling. Of major concern are nitrogen heterocycles and aromatic amines, compounds that have mutagenic potential and low odor thresholds.

(40) Additive Effects on Scrubber Chemistry
(k\$ 260)

S.G. Chang

The objective of this project is to acquire a fundamental understanding of the chemical interactions among SO_2 , O_2 , NO_x , metal chelates, and/or other additives, as well as to investigate the potential of employing metal chelates as a catalyst in a flue-gas scrubber system for simultaneous control of SO_2 and NO_x emissions. The advantage of immobilization of metal-ion catalyst onto solid substrates such as a porous glass and a cross-linked polystyrene divinylbenzene lattice attached with various chelating functional groups will be studied. This advantage could include the simplification in process design for species separation, reduction of water, energy and catalyst consumption, and reduction of operating costs. Several methods for the regeneration of ferrous chelate catalysts in the scrubbing liquors will be studied. These include the reduction of ferric chelates with solar energy, H_2S , or NH_2OH , which is a reaction product of the system.

(41) Aerosol Physics
(k\$ 200)

H. Rosen

This project will explore the role of carbon particles in atmospheric radiative transfer. Recent studies at LBL have shown the presence of large concentrations of graphitic carbon particles in urban atmospheres and in the remote Arctic region. The concentrations of these combustion-generated particles throughout the Arctic troposphere are substantial, with the concentrations in certain layers as large as those found in urban areas in the United States. Previous studies emphasized the role of aerosols as efficient scatterers of the sun's radiation and mediators of a cooling effect. These results have added a new dimension to the radiation transfer problem since the absorption coefficients associated with these black particles could be large enough to lead to substantial heating effects. We will study the optical properties, vertical and horizontal distributions, trends, and sources of carbon particles. The initial research effort will emphasize studying the Arctic haze, where model calculations indicate a significant heating effect caused by carbon particles. The influence of this heating on first detection of a CO_2 signal in the Arctic will be investigated.

(42) Unimolecular Kinetics
(k\$ 125)

N.J. Brown

Combustion chemistry consists of complex, chain mechanisms involving radical species. The inherent difficulties encountered in high-temperature environments and the large number of species involved in hydrocarbon oxidation make the study of combustion chemistry difficult. Task 1 of the current research is concerned with the application of theoretical chemical kinetics to study high-temperature kinetics important in combustion. Emphasis has been placed upon investigating the dynamics of reactions using classical trajectories. Unimolecular and biomolecular reactions are investigated with realistic potential-energy surfaces. Special emphasis has been placed upon elucidating the role of molecular angular momentum of intramolecular and intermolecular energy transfer processes. Rate coefficients for reactions important in combustion are also determined with statistical theories. Task 2 is concerned

with investigating the ignition chemistry of hydrocarbon/air mixtures. Identification of the principal elementary reaction steps that occur during ignition of hydrocarbon/air mixtures and determination of the corresponding rate coefficients are required to achieve an understanding of ignition. Initially, ignition will be investigated in a static system, and the time-resolved evolution and decay of active radical species will be monitored. Temporal measurements of radical concentrations will be achieved with a molecular-beam mass spectrometer and with spectroscopy.

(43) Ignition Studies
(k\$ 180)

A.K. Oppenheim

The principal objective of this study is the acquisition of fundamental knowledge for the development of controlled combustion systems. For the power-plant and internal-combustion-engine technologies, such systems offer the prospect of concomitantly maximizing thermal-energy conversion efficiency, minimizing pollutant emissions, and optimizing the tolerance to a wide variety of fuels. For this purpose, a thorough understanding of ignition—the initiation of a self-sustained exothermic process of combustion—is essential. Primary emphasis in this project is placed, therefore, upon an experimental study of the fundamental features of ignition. Using as the test media an assortment of lean gaseous mixtures, as well as incomplete combustion products, a variety of ignition methods are employed, including flash photolysis, electric-spark discharge, and plasma jets. The major objective of the experimental program is to determine the particular role played in the course of ignition by active radicals. The most important measurement is, consequently, concerned with their concentration histories. This is to be accomplished by the use of a high-frequency response, molecular-beam mass spectrometer that has been designed and built especially for this purpose.

(44) Laser Characterization of Pollutants
(k\$ 315)

N. Amer

The immediate task is to develop novel laser spectroscopic techniques and to employ advanced applied physics concepts for the ultrasensitive measurement of minute optical absorption and vibrational spectra of gases, liquids, and solids; the ultimate goal is to develop highly sensitive multiparameter molecular and atomic detectors of trace constituents. A subtask of this effort is the development of spatially resolved ionizing-radiation detectors. Another is the development of liquid-crystal gas analyzers.

Laser Photothermal Detection and Spectroscopy research is aimed at developing and investigating laser photoacoustic and photothermal schemes for the ultrasensitive multiparameter detection of trace constituents (molecular and atomic) in gases, liquids, and solids. Special emphasis is placed on developing *in-situ* and remote-sensing detection schemes. These sensitive laser techniques are also exploited for performing ultrahigh-resolution spectroscopy. A new activity in this subtask is the investigation of the feasibility of radiation-acoustic spectroscopy for the detection of ionizing radiation with high spatial resolution. In Liquid Crystal Physics, the research goals are to investigate liquid-crystal devices and to develop sensitive and simple personal dosimeters to detect and quantify exposures to trace organic gases. The effects of ionizing radiation on the inherent molecular order of liquid crystals are also investigated with the objective of developing novel spatially resolved ionizing-radiation detectors.

(45) Fire Modeling
(k\$ 78)

P. Pagni

The overall goal of this project is to develop physical and mathematical models of the detailed combustion phenomena that control a fire's growth within a compartment and subsequent propagation throughout a structure. Two major, coupled efforts have been completed: (1) flame height or excess pyrolyzate analyses and (2) carbon particulate volume-fraction measurements in diffusion flames. The coupling comes from the dominant role of radiation in medium- to large-scale fires. The goal of the flame-height studies was to predict the quasi-steady flame size produced by a given material in a given geometry in a real fire. To do this it was necessary to quantify the radiation feedback, controlled largely by the soot in the flame, from the flame to the pyrolyzing fuel that supports it. Now that measurements of flame soot have been completed, we are attempting to formulate an empirical model incorporating the soot formation, transport, and destruction processes in sufficient detail to predict changes into the amount of soot as the fuel, scale, and ambience of the fire are changed. Two uses of these results are envisioned: (1) incorporation of flame characteristics into compartment fire models and (2) development of valid standards to quantify the fire hazard of component materials.

**(46) Role of Primary Combustion-Generated Oxidant
in SO_2 Oxidation**
(k\$ 92)

T. Novakov

This project is concerned with certain aspects of heterogeneous aqueous-phase SO_2 oxidation. The research is based on a recent demonstration that incomplete combustion is a source of oxidants (H_2O_2 and organic hydroperoxides). This concept of primary oxidants in the context of atmospheric chemistry is quite new because it is generally assumed that all oxidants are secondary in origin. The origin of the primary oxidants is in the precombustion reactions. In situations of incomplete combustion, a fraction of these species will not be oxidized and will appear in the combustion effluent. Primary oxidants are water soluble and efficiently react with dissolved S(IV) to form sulfate. This research will proceed along two lines: (1) study of the chemical properties of the oxidant, speciation, and kinetic studies of oxidant + S(IV) + H_2O systems; (2) development of emission factors for certain sources of primary oxidants such as automobiles. The research on these topics will be studied in systems consisting of a combustor coupled to chemical reactors for chemical studies in bulk and dispersed phases.

**(47) Synergistic Effects of Metal Ions on Sulfur(IV)
Oxidation by Oxygen**
(k\$ 80)

S.G. Chang

Basic kinetic data of reactions involved in power-plant flue-gas-desulfurization (FGD) scrubbers are needed to develop a comprehensive simulation computer model for the prediction of optimum operating conditions. One important reaction, which has not been completely understood, is the oxidation of sulfite/bisulfite ion to sulfate in the presence of metal ions. Since actual operating FGD systems contain many metal impurities, the mixed metal system should be investigated to determine if synergistic effects on oxidation of sulfite/bisulfite ion occur. In this project, we study the reactions in a high-pressure rapid-mixing flow system by laser Raman spectroscopy. The system allows the measurements of fast oxidation rates of S(IV) by oxygen resulting from the catalytic effects of metal ions at concentrations comparable to those of realistic FGD scrubbers. Also, this system can provide high concentrations of dissolved oxygen and may allow the detection of some intermediates and products present during the progress of reactions. The information obtained will be used to identify reaction mechanisms and to provide accurate basic kinetic data for the development of a FGD process-simulation computer model.

(48) Mitochondrial Free-Radical Detection
(k\$ 103)

R. Mehlhorn

Electron spin resonance methods for free-radical detection will be used to study one aspect of the hypothesis that oxygen radicals generated during normal metabolism cause mammalian aging (free-radical theory of aging). The research will focus on mitochondria, the components of cells that use nutrient combustion to meet cellular energy needs. During this combustion process, unavoidable free-radical processes liberate destructive oxidants that have the potential to wreak havoc throughout the cell. We will quantitate the production of these radicals, determine where they are generated and how they propagate to distant targets, and characterize their subsequent reactions with membranes and proteins. The study will use nitroxide spin labels, developed in our laboratory over the past few years, as free-radical "traps" to quantitate the occurrence of such radicals within specific domains of mitochondria. Nitroxides will also be used to study membrane surface architecture during the course of free-radical attack so that damage sites can be identified.

(49) Nitrogen Recycling in a Closed Life-Support System
(k\$ 40)

L. Packer

This project proposes to determine conditions for the most efficient reduction of N_2 gas by cyanobacteria (blue-green algae) so that they can be effectively exploited as a source of combined nitrogen. We will screen strains and select for study those that appear to be particularly suitable for long-term culture, hardiness, and activity.

The bioenergetics of N_2 fixation will be studied. The approach will employ new specific and sensitive spin-labeled probes that enable us to measure the significant bioenergetic parameters of pH, membrane potentials, volume, and reducing power under very nearly identical conditions inside cells with electron spin resonance instrumentation. The influence of H_2 gas, light, organic substrates, and O_2 on N_2 fixation and on the two main components of the proton motive force—proton gradients and membrane potentials—will be studied. We will employ specific reagents known to affect bioenergetic parameters ($\Delta pH, \Delta \Psi$) and explore ways of enhancing the uptake activity of hydrogenase to increase N_2 reduction to ammonia.

Substances known to act at low external concentrations to inhibit nitrogen assimilation will be used to investigate partitioning of ammonia and other products of N_2 fixation between the surrounding medium and biomass.

(50) Life Extinction
(k\$ 27)

F. Asaro

Samples have been collected from 19 continental sites in Western North America, and most of these will be scanned for Ir in the next year. The purpose of these studies is to ultimately provide a high-precision stratigraphic time marker for continental Cretaceous-Tertiary (C-T) studies.

An intensive search for 34-million-year-old microtektites in Italian Apennine rocks (such as found in deep-sea cores) has been fruitless. We propose to scan 80 samples for Ir covering about 1/4 of a 16-meter Contessa-Barbetti section at Gubbio, Italy known to contain the Eocene-Oligocene (E-O) boundary.

If we can find the Ir anomaly in the 16-meter section, it will pinpoint the relative stratigraphy of this area with respect to the deep-sea cores where 34-million-year-old microtektites have been found. We will use a new measurement technique that we have developed in which Ir is nearly quantitatively removed from silicate samples with molten iron in a reducing environment. Since no Ir carrier is used in this separation, the problems of contamination are

reduced.

(51) Energy Efficiency in Buildings in ASEAN Countries
(k\$ 39)

M. Levin

This project, funded by the U.S. Agency for International Development (USAID) through DOE, will investigate the state of energy used in commercial buildings in the ASEAN (Association of South East Asian Nations: Singapore, Philippines, Thailand, Malaysia, and Indonesia) in which energy use has been growing very rapidly during the past ten years. Much of the information, research, and technology that could ameliorate this trend has been developed in the U. S. during the past years and can form the basis for application in ASEAN circumstances. Application of the experiences gathered in the U. S. in energy and use analyses, data-base compilation, computer energy-use programs, technologies, and design for energy-efficient retrofit as well as new building application will form the basis of an assistance program that would be of benefit to all the ASEAN countries. This project is an outgrowth of a visit by Sam Berman to Singapore at the request of USAID. As is common with USAID projects, the project is still not well defined but will become so in interaction with the host country. We anticipate that in the first year the emphasis will be on technical issues related to DOE-2 and that in the second year the emphasis will shift to more policy-oriented issues.

(52) Building Analysis
(k\$ 1090)

R.L. Ritschard

The objective of this research is to analyze factors affecting energy use in buildings to: (1) increase understanding of whole-building performance; (2) develop simplified analysis tools to evaluate building energy efficiency and to further knowledge of interactions among climate variables, building characteristics, occupant behavior, and energy use; and (3) support DOE policies for voluntary performance guidelines and standards. The LBL program is focusing on the following areas:

1. *Multi-Family Research.* Perform energy analyses for low-rise multi-family buildings in various climates and develop design and system recommendations that are applicable in specific climate regions.
2. *Regional Residential Research.* Develop simplified design tools and guidelines for architects and builders that are applicable in specific regions. The research will be aimed initially at reducing cooling loads in hot climates.
3. *Design Factors Research.* Gain better understanding of critical building parameters and interactions of conservation measures that influence energy use in different climates.
4. *Technical Support for Standards/Guidelines.* Provide technical, energy, and economic analysis in support of DOE's building-energy performance standards and guidelines.

(53) Appliance Studies
(k\$ 714)

M. Levine

The objective of the work is to support DOE's legislatively mandated reanalysis of energy-efficiency standards for consumer products. The work will provide a continuing and improved analytic basis for DOE to draw upon in the legislatively mandated reanalysis of appliance-efficiency standards. It will also provide the analysis for the proposed rulemaking for the three products that have been treated as "space reserved": heat pumps, home heating

systems, and heat-pump water heaters. Improvements to the LBL Residential Model will be made following the recommendations of the Analytic Review Group. Additional data will be collected for the reanalysis of standards. LBL will continue managing technical programs in support of the DOE analytic activities.

(54) Residential Conservation
(k\$ 185)

L. Schipper

In Part 1, we will complete the Organization for Economic Cooperation and Development (OECD) Residential Energy Analysis begun in FY 1979 by adding two or more European countries, updating Japanese and United Kingdom data to CY 1982, and completing the comparison of end-use indicators. Results will be integrated into our residential energy use data base and tested with the econometric models developed in FY 1982. We will extend and document our analysis of energy use in commercial buildings. We will complete our comparison of electric appliances in the major countries of the study.

In Part 2, we will complete a user-oriented data base with documentation of all of our residential (and commercial) energy-use data. Publications will describe the important aspects of our overall findings, such as changes in heating fuels and electric appliances, changes in use patterns, and energy intensities of new homes and appliances compared with older ones.

In Part 3, we will analyze foreign buildings conservation efforts. These will include the overall achievements in Sweden, the new laws on building energy use in Denmark, the National Insulation Program in Holland, and the Canadian Home Improvement Program. We will judge overall U.S. performance *vis à vis* these nations, given our information on consumption, price, and income through CY 1983.

(55) Energy Demand in Developing Countries
(k\$ 155)

L. Schipper
J. Sathaye

This project will continue important efforts in collecting and analyzing energy-consumption information from less developed countries (LDC's) begun in FY 1982. The methods developed in earlier studies will be used to collect and analyze data in 20 LDC's that account for most of the non-OECD (Organization for Economic Cooperation and Development) oil imports, as well as in four large oil-exporting countries.

This project will present a complete analysis of 15+ LDC's, including a detailed description of each sector over time; a review of important trends in structural change and composition, conservation, and fuel switching; and a study of key topics in selected countries. The output of this study will include a computerized data base on LDC energy use and structure. Additionally, analysis of 15 African countries will be started in FY 1985.

BIOLOGY AND MEDICINE DIVISION

E.L. Alpen, Associate Director

- (1) **Lipoprotein Methodology and Biomedical Applications**
(k\$ 1,527)

F.T. Lindgren

This research program continues to focus on serum lipoproteins considered as biochemical entities of significance in the etiology of atherosclerosis, lipid disorders, and other diseases. Understanding such relationships requires the elucidation of the chemical, physical, and functional characteristics of the lipoproteins. Our research therefore emphasizes detailed characterization, as well as quantification, of serum lipoproteins in terms of classes and subclasses, distributions, interrelationships, and origins. Our investigations of the lipoproteins will address a variety of problems and employ a broad scope of experimental techniques and skills. Among the principal tools that we expect to develop and apply to fundamental biophysical and biomedical problems are: analytic ultracentrifugation, electrophoresis, electron microscopy, chromatography, enzymatic methods, computer technology. An apolipoprotein core unit is directed toward determination of specific apolipoproteins. Lipoprotein structure and function will be examined in native and partially degraded particles and in physical or enzymatically reassembled model structures. Transformation in lipoprotein distributions will be studied *in vitro* as well as *in vivo*; the latter as a function of diet, drugs, and disease. Human umbilical-cord blood will be analyzed for information and insights into the genesis of lipoproteins. A major methodologic effort is concerned with detection and minimization of potential artifacts and degradation arising from lipoprotein isolation and analysis. The unique methodologic resources of this Program Project will be available for outside collaborations on specialized or unique biomedical problems. The interactive design of developing methodology with application to basic and clinical research problems remains a major feature of our Program Project.

- (2) **Factors Regulating Hemopoietic Progenitors in Marrow**
(k\$ 90)

J.W. Goodman

It is generally agreed that T lymphocytes are involved in regulating blood formation, although data from *in-vitro* experiments do not give a consistent or quantitative description of the regulation and its underlying mechanisms. Even less is known about the regulation of marrow stem cells that are committed to the T-lymphocytic pathway. *In-vivo* experiments are proposed here that will test the ability of lymphocyte depletion, by means of ATS injection, and plethora, resulting from T-cell transfusions, to modify (in a pseudo-physiologic manner) lymphocyte progenitors in the bone marrow. Ability of marrow that has been subjected to lymphocyte depletion or plethora to repopulate thymus and to restore immune function will be determined *in vivo*. Using purified interleukins (IL-1, IL-2, IL-3, and possibly others) we will try to develop a simple short-term culture method, based on our previous experience, to permit enumeration of pre-T cells in marrow. From pre-T colonies growing *in vitro*, subculturing and cloning will be carried out. Finally, studies will be initiated to examine the role of purine nucleosides in progenitor regulation by T lymphocytes. *In-vitro* studies will explore metabolic and surface membrane receptor modes of activity, and *in-vivo* studies will be based on results of those experiments.

(3) Kinetics of Transfused Stem Cells
(k\$ 73)

G. Brecher

The approach to the study of pluripotential stem cells is based on the recently demonstrated successful transfusion of bone marrow into normal, nonirradiated recipients. The studies have been greatly aided by the use of a new strain allowing electrophoretic determination of donor and host cells on periodic examination of the peripheral blood. We propose to culture pluripotential and committed progenitor cells to follow their time course *in vivo*. Using the same approach we hope to resolve the question whether the variable proliferation of transfused marrow cell is due to variation in the initial proliferation of stem cells or varying delays in differentiation. We propose to follow up indications, obtained in our laboratory, that transfusion itself is deleterious to self renewal of marrow cells. We shall perform serial transplants of bone marrow at slightly different doses of irradiation to quantify the role of radiation in the process. We shall follow up preliminary indications that platelet production from donor cells lags behind red-cell production.

The studies should contribute to our understanding of proliferation and differentiation of transfused marrow cells. The serial transfer studies may possibly have bearing on the controversy relating to the Hayflick phenomenon.

(4) Vascular and Blood Diseases
(k\$ 315)

S.N. Ebbe

Reactions of blood platelets with blood vessels and production of platelets will be evaluated. Important cellular relationships in these processes should be demonstrable with the application of new technology.

Platelet vessel-wall interactions will be evaluated by positron emission tomography (PET). Blood platelets will be labeled, and their distribution will be determined in normal and in damaged blood vessels. Development of methodology for rapidly processing platelets for labeling is under way. The demonstration of platelet adherence to damaged vessels by PET would provide a new capability to repeatedly monitor the progress of an individual patient's vascular disease and to analyze the pathogenesis and treatment of atherosclerosis and, perhaps, small-vessel diseases.

We have demonstrated that abnormalities of megakaryocytopoiesis *in vivo* can be reproduced in marrow cultures. Cultures of murine bone marrow cells will be evaluated for relationships between megakaryocytes and marrow stromal cells and for regulation of megakaryocyte precursor cells. Identification of relationships between stromal cells and megakaryocytes and analysis of behaviors of precursors should improve the understanding of the regulation of megakaryocytes, their role in some types of bone-marrow failure, and the origin of platelet factors that may play a role in vascular diseases.

Future studies will apply the results of these experiments to other models of vascular diseases and to human vascular diseases. The use of labeled soluble coagulation factors for PET imaging of vascular diseases will be considered. Cell-culture results will be correlated with hemopoiesis *in vivo*. Studies of blood flow to the bone marrow (microspheres, nuclear magnetic resonance) will be added.

(5) Kinetics of Megakaryocyte and Platelet Turnover
(k\$ 182)

S.N. Ebbe

The long-term objective is a better understanding of the ways in which the production of blood platelets is regulated. It is well known that the level of platelets in the blood regulates megakaryocytopoiesis, but there is an increasing amount of evidence that megakaryocytes are probably also regulated by other factors. The hypothesis being tested in the proposed experiments is that the number of megakaryocytes themselves may, in part, regulate megakaryocytopoiesis. Conditions characterized by megakaryocytopenia with normal (or disproportionately high) platelet production will be studied and compared with experimentally induced thrombocytopenia with intact marrow and also compared with conditions in which both megakaryocytes and platelets are low. Measurements will be made of megakaryocyte size, DNA content, and number; total marrow cells; and blood platelets, red cells, and white cells. Liquid cultures of marrow cells will be made to detect abnormalities of hemopoietic stromal cells. Megakaryocyte-colony-forming cells will be measured in an effort to evaluate their physiological role *in vivo*.

(6) Radioassay of Erythropoietin
(k\$ 112)

G.K. Clemons

Erythropoietin is now accepted as the hormone controlling red blood cells production. A radioimmunoassay has been developed in this laboratory using pure radioiodine-labeled erythropoietin and an antierythropoietin antiserum. This assay measures not only normal circulating levels but also depressed levels seen following physiological conditions known to depress erythropoiesis and following increased hormone levels associated with stimuli known to increase erythropoiesis, such as bleeding, hypoxia, or cobalt administration. This radioimmunoassay shows a significant correlation with several bioassay systems. Using this method, polycythemia of primary origin are distinguishable from those of secondary origin. The clinical significance of this study is derived from the diagnostic value of a sensitive radioimmunoassay for blood levels of erythropoietin. Clinical work in this study deals with erythropoietin responses to controlled stimuli, which may ultimately be of value diagnosing increased or decreased secretory ability. Fetal hypoxemia in high-risk pregnancies can be diagnosed by measuring the hormone levels in the amniotic fluid. In addition to human erythropoietin, a variety of other erythropoietins are measurable with this assay. Some of the work is concerned with both the production of erythropoietin and the mechanism of action on its target tissues. The role of this hormone in fetal and neonatal erythropoiesis, as well as site of production and concentrations as a function of age, will be investigated. Other studies are concerned with the effects of other hormones on erythropoietin synthesis and release and with extrarenal sources of erythropoietin. The effort to produce antibodies with higher affinity will continue. Monospecific antihodies will be isolated and used in morphological studies of the sites of erythropoietin production. Also, studies are proposed relating to the development of a radioreceptor assay for erythropoietin. A radioreceptor assay in conjunction with the radioimmunoassay will give a new dimension to the importance of erythropoietin detection in clinical studies. The knowledge gained from this investigation will add significantly to our understanding of the biogenesis and mechanism of action of erythropoietin and of the role of this hormone in normal and diseased states in humans.

(7) Yeast Rad Genes in Repair, Recombination, and Meiosis
(k\$ 187)

R.K. Mortimer

We will characterize the nature and interrelationships of repair, recombination, and meiosis in the yeast *Saccharomyces cerevisiae*: the exact role of DNA repair (*RAD* genes in normal cell metabolism, including mitotic and meiotic recombination, as well as how they function in DNA repair). We will study those current and new *RAD* genes whose mutants

confer sensitivity to x rays, since it is primarily these mutants that show complex phenotypes involving normal mitotic or meiotic DNA metabolism as well as repair. *Genetic Studies:* Recently isolated *rad* mutations will be examined to see if they define new *RAD* loci. To determine if any of the existing *RAD* genes code for essential functions, we will isolate both deletions and nonsense alleles by *in-vitro* mutagenesis with cloned genes. Reversion studies on some of the *rad* mutations will be done to isolate new temperature-conditional and regulatory alleles and to determine if the *RAD* gene products interact with each other or with other proteins. We will continue our studies on chromosome loss in existing *rad* mutants. *Meiotic Studies:* We plan to study the meiotic defects of the *rad* mutant to learn more about both the *RAD* gene products and the process of meiosis. We will perform temperature shifts on double-mutant strains containing heat-sensitive and cold-sensitive alleles. We will also study strains containing *rad* mutants in combination with meiosis-I by-pass mutations. These approaches, in combination with transcriptional studies, will provide information about dependent sequences and the order of gene functions in meiosis, as well as the timing of various stages of recombination and their relationship to other aspects of the meiotic divisions. *Molecular Studies:* Using already isolated clones of six *RAD* genes, we will determine if and when these genes are transcribed during meiosis and whether they are induced by DNA-damaging agents in mitotic cells. Using high-expression vectors and nuclear isolation procedures we will attempt to isolate and characterize the *RAD* gene products.

(8) Comparative Analysis of Mitotic and Meiotic Recombination
(k\$ 148)

M.S. Esposito

Our research program involves the genetic and biochemical characterization of 20 *rec* mutants of *Saccharomyces cerevisiae*. The mutants comprise five phenotypic groups with respect to enhancement (hyper-recombination) or depression (hypo-recombination) of gene conversion and/or intergenic recombination. The collection will be characterized with respect to the number of *REC* gene loci involved by complementation and meiotic segregational analysis. Representative mutants from each phenotypic group will be examined for their effects upon mitotic and meiotic recombination. Protein extracts from mutants will be characterized with respect to known yeast exonuclease and endonuclease activities. Biochemical studies will include analysis of mutants for presence of single-stranded DNA binding proteins. The *REC336* gene product has already been shown to be necessary for binding of several acidic nonhistone proteins to DNA.

(9) Genetic Study on Yeast
(k\$ 200)

R.K. Mortimer

The yeast *Saccharomyces cerevisiae* is currently being studied in a large number of laboratories as a model eucaryotic cell. The mitotic and meiotic cycles of this organism are typical of higher eucaryotes as are the processes of DNA replication, transcription, and translation. Remarkably, it has very recently been shown that several mammalian oncogenes show close sequence homology to particular yeast genes, some of which control the cell cycle. This argues for a strong conservation through evolution of critical genes. Thus, studies on yeast, which is very tractable to both genetic and molecular investigations, should be of great importance for understanding higher eucaryotic cells.

Our laboratory has worked on yeast for many years and over much of this time we have worked on developing the genetic map of this organism and are continuing to do so. We have also carried out many studies on suppressors and on the radiation genetics of this organism. Currently we are concentrating on a group of genes involved in recombination! repair of DNA lesions. Mutations in these genes result in x-ray sensitivity, mitotic instability, and recombination deficiencies. We are using genetic and recombinant-DNA techniques to determine how these genes are regulated and to identify their products. The eight genes in this series, *rad50-57*,

were identified mostly in our laboratory, and these genes have been characterized genetically and phenotypically over the past 15 years. One of these genes, *rad52*, has been widely used because of its pronounced effects on recombination and double-strand break repair. We are using nuclear isolation procedures and high-expression vectors to study the products of these *rad* genes and Northern procedures to study their regulation.

(10) Mitotic Recombination and DNA Repair
(k\$ 75)

M.S. Esposito

Objective. The primary objective of the research is to determine the mechanisms of mitotic recombination and the molecular defects of yeast strains containing mutant *REC* genes.

Approach. Recombination occurring spontaneously and after exposure of mitotic cells to recombinagenic treatments is assessed genetically and by electron microscopic visualization of recombinant DNA plasmids. Previously isolated *rec* mutant strains are employed for molecular cloning of *REC* genes and are characterized with respect to stages of the recombination process in which they are defective.

Expected Accomplishments. Previous research has provided strong evidence that both spontaneous and recombinagen-induced mitotic recombination occur by mechanisms that differ from those that occur in meiotic cells. We expect that the studies proposed will provide tests of molecular models and a better understanding of the recombinational pathways of eukaryotes.

Implication of Accomplishments. An understanding of the pathways of recombination in eukaryotic species is a point of departure for a critical evaluation of the role of genomic rearrangements in the control of gene expression during development and in differentiated cells.

(11) Carcinogenic DNA Damage
(k\$ 40)

P.K. Cooper

DNA in living cells is continually subject to a variety of deleterious alterations, both spontaneous and induced by external agents. A variety of enzymatic processes are employed by cells to repair or lessen the impact of such DNA damage, most of which appears to be both mutagenic and carcinogenic as well as potentially lethal. Some of these processes are not constitutive but are induced in response to the damage itself. The objective of these studies is to understand such induced responses, with emphasis on the apparent dichotomy between processes affecting survival and those affecting mutation. *Escherichia coli* is used as a model cell system because of the availability of relevant mutants and extensive genetic and biochemical characterization. Quantitative measurements of repair-DNA synthesis by combined radioisotopic and density labeling in normal cells and in mutants deficient in one or more known repair functions are employed together with analysis of cellular survival and replicative-DNA synthesis.

Our previous investigations have identified and characterized long-patch excision repair of ultraviolet irradiation damage in *E. coli* and shown it to be one of the inducible "SOS processes." We have shown that the major component of the enhanced cellular resistance produced by induction of SOS functions irradiation is a *uvr⁺*-dependent process that correlates with long-patch repair. The evidence suggests that long-patch repair occurs at a particular small class of damage sites, perhaps lesions in functionally distinct regions of the genome, that are potent blocks to replication and that cannot be repaired by the constitutive process. These findings provide a unique basis for investigating the molecular mechanism by which induced responses can increase resistance to damage. Whether removal of critically situated lesions is involved or whether an incision-initiated event contributing to tolerance of damage is responsible will be of particular interest.

Improved understanding of the mechanism of these processes and of the interaction between them and others that primarily affect mutagenesis is ultimately necessary for understanding the potential for carcinogenesis and cumulative lethal effects of long-term exposure to low levels of environmental DNA-damaging agents.

(12) DNA Repair Mechanisms
(k\$ 32)

J. Hosoda

The goal of this study is to elucidate mechanisms controlling complex repair pathways generally called recombinational and/or error-prone repair and to find their relationships to DNA replication, mutagenesis, and carcinogenesis.

We have proposed that gene 32 product, a single-stranded DNA binding protein (ssb) of bacteriophage T4, has domains specifically assigned for the control and coordination of proteins involved in DNA metabolism. In the last few years we were able to show that: (1) the majority of known T4 repair-gene products have an affinity for T4 ssb; (2) the intact carboxy terminus region A (about 50 residues) seems essential for such affinity; (3) a mutant in gene 32, *amel*, which has an elevated UV sensitivity and a reduced recombination rate, produces a protein lacking about half of the A region; and (4) the *amel* protein has no affinity for *uvsX* and a reduced affinity for *uvsY* (*uvsX* and *uvsY* are two of the major genes in the T4 error-prone repair pathways, and both have strong affinity for the intact ssb). In addition, using the T4 ssb-affinity chromatography, we were able to purify the *uvsY* gene product from a cloned bacteria and to begin its characterization.

We plan to continue identification, purification, and characterization of T4 repair-gene products and determination of their interactions with the ssb. We also plan to extend the "ssb-controlled repair protein model" to eukaryotic systems, the immediate targets being the repair pathways and the ssb of *Saccharomyces*. A preliminary analysis of yeast DNA-binding proteins by two-dimensional gel electrophoresis is in progress.

(13) The Structure of Helix-Destabilizing Protein
(k\$ 248)

J. Hosoda

The objective of this research is to study the structure of bacteriophage T4 gene-32 product, a helix-destabilizing protein, and to examine its roles in DNA replication, recombination, and repair. The specific aim of this proposal is to elucidate interactions of 32 protein with itself and those with other proteins and understand how such interactions control and coordinate the activities of individual enzymes and to elucidate the overall structure and activities of the replication-recombination complex.

Some years ago, we started a line of research using limited proteolysis products of 32 protein to correlate the structure and the functions of the protein. The results indicated that 32 protein has several discrete domains, and some of the domains seemed to be specifically involved in protein-protein interactions. We plan to continue this line of research with expansion to include mutationally and chemically modified protein research with intensified structure studies.

Proposed experiments consist of preparation of various 32-protein fragments and mutationally or chemically modified proteins; chemical and physical studies to examine their structure and that of their macromolecular complexes; extensive use of 32-protein affinity chromatography to examine protein-protein and protein-DNA interactions as well as identification of 32-binding proteins; mapping of the contact area and detection of conformational changes by differential chemical modification; and use of 32-protein fragments and modified proteins in *in-vitro* replication reactions to correlate the physical interactions with the functional ones.

(14) Physical Structure of Viruses, Chromosomes, and Cell Nuclei
(k\$ 290)

M.F. Maestre

The main objective is to study the structure of viruses, nucleoproteins, and chromosomes. Particular emphasis is on the internal organization of their nucleic acids. This will be attempted by using the remarkable optical properties of both DNA and RNA in their various chemical and physical states (charge, single or double strandedness, secondary and tertiary geometry alteration in aggregates and in protein complexes, etc.).

The most important methods will be: (1) circular dichroism (CD) and flow oriented CD; (2) circular dichroic microspectrophotometry; (3) electric and flow dichroism, electric and flow birefringence; (4) fluorescence-detected circular dichroism (FD CD); and (5) scattered corrected CD by fluoroscat and FD CD.

The above techniques will give information concerning the following properties: (1) the interactions between the bases of the nucleic acids, the nucleic acids and protein complexes, and the protein components with themselves in such biological structures as viruses, chromosomes, and intact nuclei; (2) the electric and hydrodynamic properties of the protein coats and the average orientation of nuclei acids in viruses, nucleoproteins, and chromosomes; and (3) the superorganization of nucleic acids in viruses, nucleohistone-DNA and RNA aggregate and/or complexes, and the degree of coiling of nucleic acids in intact nuclei and intact cells.

With the help of the above measurements and the recently developed theory of circular intensity differential scattering (CIDS), it is possible that models satisfying all the measurements can be constructed, thus giving insight into the organization of nuclei acids in biological structures, and that through this research, new optical diagnostic techniques can be developed for detecting the identifying viruses, normal and abnormal cells in cancer cytological studies, and the state of the chromosome through its life cycle in the intact nuclei.

(15) Rapid Transformation Assay
(k\$ 89)

M.R. Stampfer

Our objective is to develop a protocol for detecting carcinogen-induced transformation *in vitro* of human mammary epithelial cells (HMEC) that can be used as a simple, rapid quantitative assay for determining what agents alone, or in combination, may be capable of inducing human carcinoma.

Previous work in our laboratory has led to the development of a well-characterized HMEC culture system that has provided most of the prerequisites for achieving transformation *in vitro*. We have a large bank of frozen primary cells from donors of all ages and pathologies that allows repetition of experiments with the same cell population; the normal HMEC can be made to proliferate rapidly, both in mass culture and as colonies, up to 20 passages (the cells have markers that identify them as mammary and epithelial); the HMEC have been shown to rapidly metabolize benzo(a)pyrene (BaP), forming products and DNA adducts in a pattern similar to that found in cells transformable *in vitro*; we have begun to identify tumor-associated markers for the HMEC that may permit quantitative selection and detection of transformed cells. With the identification of properties that distinguish tumor cells from normal cells, we can now attempt to induce expression of these properties by exposure to BaP alone or in conjunction with other suspected co-carcinogens and promoters (e.g., radiation, fatty acids, phorbol esters, hormones).

Our results thus far have been very promising. BaP is consistently able to induce extended life in cultures of HMEC. At least two BaP-induced cell lines have been developed, with properties that distinguish them from normal cells (morphology, karyology, expression of specific antigens, glucose metabolism, x-ray sensitivity). We hope that some of these differing

properties will allow us to quantitate the frequency of carcinogen-induced changes *in vitro* so that the ability of different agents to induce, or inhibit, transformation can be determined.

(16) Effects of Benzo(a)pyrene (BaP) on Humans
(k\$ 70)

J.C. Bartley

Our overall objective is to determine if polycyclic aromatic hydrocarbons (PAH), BaP in particular, could be factors in the initiation of breast cancer and, if so, can PAH metabolism be modulated in ways that would increase or decrease the yield of the ultimate carcinogen and, thereby, the risk of malignant transformation. We have demonstrated that, compared to fibroblasts, human mammary epithelial cells (HMEC) readily metabolize BaP to the ultimate carcinogen and that the extent of DNA modification is similar to that in cells transformable by BaP, an indication that PAH should be included as possible factors in the initiation of breast cancer. Our initial studies on modulation of BaP metabolism used polyunsaturated fatty acids (PUFA) because of the experimental and epidemiological evidence for a relationship between dietary PUFA and the risk of breast cancer. Linoleic acid, the precursor of arachidonic acid and prostaglandins in the cell, specifically stimulated overall BaP metabolism, but the greatest increase was in the yield of the most carcinogenic form of BaP diol epoxide. An inhibitor of prostaglandin synthesis blocked this effect. These results provide a partial explanation for our initial findings: the enzymes of prostaglandin synthesis supplement the usual epoxidation by aryl hydrocarbon hydroxylase and, thereby, contribute in HMEC both to the initial oxidation resulting in formation of the dihydrodiol and, to an even greater extent, to the conversion of the dihydrodiol to the ultimate carcinogen. These results, in addition to portraying the pathway of conversion of BaP to the ultimate carcinogen in HMEC, may have direct medical significance. The supplementation of BaP diol epoxide formation resulting from the presence of the prostaglandin enzyme complex in epithelial cells would provide a partial explanation for the relationship between diets rich in PUFA and the incidence of breast cancer and may help explain the particular risk of certain human epithelial cells to initiation of malignancy (breast, colon, prostate).

(17) Monoclonal Antibodies
(k\$ 78)

G. Parry

We plan to investigate the organization and the biosynthesis of glycoproteins at the surface of mammary epithelial cells. The research will form a basis for analysis of the surface organization of glycoproteins on normal and tumor epithelial cells and has implications for a better understanding of tumor-cell heterogeneity and metastasis, as well as for a basic understanding of cellular differentiation.

The surface of normal mammary epithelial cells is polarized in that it is organized into two distinct domains, an apical domain and a basolateral domain. The apical surface faces the milk duct, and the basolateral surface faces the blood vessels. The composition of these domains appears to be different in that the apical surface contains some components destined for milk, whereas the basolateral surface is composed of basal lamina components, transport proteins, and glycoprotein receptors. We plan to study how these polarized domains are maintained as organized units, how they are synthesized and assembled, and how the organization is altered in tumor cells.

Our approach will be to prepare polyclonal and monoclonal antibodies against specific components of these domains and to use them to follow biosynthetic routes and to investigate the factors responsible for maintaining membrane polarity. Specific emphasis will be placed on studying the role of extracellular matrix components in maintaining polarity. The studies will be carried out on mouse mammary epithelia isolated from pregnant mice and on human mammary cell lines and strains.

To date we have generated a polyclonal antiserum against isolated apical membrane fragments that reacts with cultured human mammary carcinoma cells. We have also generated a series of monoclonal antibodies that react with a high-molecular-weight component of human milk fat globule membranes and are currently screening its reaction with human cells. In addition we have carried out related, nonimmunological studies with mouse cultures and have characterized a cell-culture model that mimics glandular differentiation.

(18) Characterization of Human Mammary Cells
(k\$ 141)

M.R. Stampfer

The goal of this research is to gain an understanding of the mechanisms and etiology of breast carcinoma by looking for transformation *in vitro* of human mammary epithelial cells (HMEC). We have used benzo(a)pyrene (BaP) as our initiating chemical carcinogen in these transformation studies. Our results thus far with one individual have shown that exposure of rapidly growing primary cultures of HMEC to BaP consistently leads to cell populations with extended life in culture and rarely leads to immortalized cell lines. Our objectives for the next year will include further characterization of the extended-life cultures and cell lines developed so far and extension of this work to cells from another individual. Specifically, the characterizations we plan to do include:

1. Examination of cell surface properties by both ultrastructure [scanning electron microscope (SEM), transmission electron microscope (TEM)] and gel electrophoresis analyses after labeling with fucose, ³⁵S-methionine, and lactoperoxidase-catalyzed iodination.
2. Further studies of karyology, expression of specific antigens, glucose metabolism.
3. Selection of nutritional variants (e.g., cells no longer requiring insulin, EGF, or hydrocortisone for growth), assay for possible synthesis of tumor growth factors, cell fusion experiments between normal and immortal cell lines.
4. Further treatment of extended-life cultures with carcinogens and/or promoters.
5. Assays for possible involvement of oncogenes in the transformation process (e.g., transfection experiments, analysis of known oncogenes in the DNA or expressed in RNA).

(19) Extracellular Matrix and Epithelial Lumen Morphogenesis
(k\$ 49)

H.G. Hall

This is a study of the role of the extracellular matrix (ECM) in directing epithelial-cell polarity and morphogenesis. I have developed a system in which cultured epithelial cells, growing on a substratum of type I collagen, are induced by an overlay of additional collagen to reorganize to form lumina. Several ECM components, including collagen, have been found to be ineffective in inducing lumen formation in a soluble or suspended form. Therefore, they will be coupled to dextran polymers, as outlined in the original proposal, to test if they must be in a polymeric or gel-like form to induce lumen formation. A major effect of the overlaid collagen may be on cytoskeleton organization. Upon cell lysis, cell proteins labeled with ³⁵S-methionine remain attached to the collagen gels. Most of these proteins, analyzed by two-dimensional gel electrophoresis, have now been identified as cytokeratins or actin, which may have a transmembrane association with the collagen mediated through plasma membrane proteins. Other proteins seen attached to the collagen may be either such membrane proteins or cell-synthesized matrix components. Their identification as one or the other will be attempted through selective detergent solubilization, by proteolytic treatment of the cell exterior, by radioiodination, and/or by label-transfer reagents. Preliminary experiments have shown a

difference in cytoskeletal components attached to the upper and lower collagen gels. This will be pursued in greater detail by labeling cells before collagen overlay with ^{35}S -methionine and following the distribution of the cytoskeletal proteins at different times after overlay. Labeling cells during certain time periods after overlay will be continued also. Such experiments should reveal more of the dynamics of the synthesis and polarization of structural elements during the course of lumen formation. Changes in the distribution of the cytokeratins will also be explored through immunolocalization of cross-sectioned cells both at the light- and electron-microscopic levels. Cortisol in serum-free defined media has been found necessary for lumen formation and will be used to modulate lumen formation and follow associated cell activities. Glycopeptides or a glycosaminoglycan, perhaps hyaluronic acid, separated by ion exchange, decreases in the absence of cortisol. Identification of the glycosaminoglycan as hyaluronic acid will be attempted through hyaluronidase digestion. A two-dimensional separation method we have developed will be used to resolve the sulfated glycosaminoglycans to determine if they are affected by the absence of cortisol.

(20) Biological Effects of Magnetic Fields
(k\$ 420)

T.S. Tenforde

Magnetic field interactions, and their underlying mechanisms, are being evaluated in experimental animal systems and in tissue and cellular systems that are potentially sensitive to this form of nonionizing radiation. Baseline data are being obtained for the establishment of magnetic field exposure guidelines at industrial and research facilities, including several newly developing energy technologies. This study is also related to the potential health effects associated with the use of *in-vivo* nuclear magnetic resonance for medical imaging.

The three principal areas of this programmatic effort are as follows: (1) Physiological performance in exposed mammals is being evaluated from measurements of metabolic parameters, core body temperature, activity, and neurobehavioral parameters and specific functions associated with the cardiac, neural, visual, immunological, and hematopoietic systems. Circadian variations are being monitored noninvasively as an index of stress imposed by magnetic field exposure. (2) Electrophysiological techniques are being used to study selected organ and tissue systems that may exhibit sensitivity to magnetic field as the result of electrodynamic interactions with ionic conduction processes. Two well-defined effects of stationary magnetic fields up to 2 Tesla have been characterized: (a) the induction of electrical potentials at the millivolt level within the central circulatory system and (b) the suppression of retinal electrical activity elicited by photon absorption. These effects, however, have not been found to produce functional impairment in the cardiovascular or visual systems. (3) A new series of investigations at the cellular and tissue levels was initiated during the second half of FY 1984 to characterize the bioeffects of stationary magnetic fields up to 9 Tesla. These studies will be of fundamental mechanistic value for the development of theoretical models of magnetic field interactions with biological systems and will also provide essential data for assessing the potential health effects that may result from the use of ultrahigh magnetic fields in medical applications of nuclear magnetic resonance.

(21) Assess Indirect Effects of Carbon Dioxide
(k\$ 375)

M.R. White

Atmospheric carbon dioxide (CO_2) is increasing principally because of use of the fossil fuels. It has been predicted that this increase will result in global warming with consequent regional and seasonal climate changes.

The aim of the DOE's Carbon Dioxide Research Division Program is to develop a sound quantitative understanding of the CO_2 issue for input into the energy policy-making process. The study of indirect effects, principally caused by climate change, is a part of this program.

The principal investigator for this study, working with the DOE Program Manager, will plan, manage, and coordinate field studies and research on the indirect effects of CO₂. The objective of these studies is to identify, characterize, define, and eventually evaluate the impacts of the indirect effects of increasing atmospheric CO₂ and the probable consequences to human health and welfare.

Technical reports, based on current knowledge, will be completed in the spring of 1985. These will define the knowns, unknowns, and uncertainties regarding the possible effects of tentatively predicted CO₂-induced climate changes on some critical aspects of human health and welfare. They will also outline information and research needed to reduce uncertainty about these effects. These reports will form the background for a state-of-the-art report (SOA) on indirect effects of CO₂, to be extensively reviewed and completed by January 1985. Information from the SOA will be used by DOE to prepare a statement-of-findings report for Congress in 1985 and to assist DOE in planning a CO₂ research program for the future.

(22) Hematopoietic Cell Proliferation
(k\$ 315)

J.C. Schooley

We have utilized the Dexter *in-vitro* system of bone marrow culture with Greenberger's hydrocortisone addition to quantify changes in murine stromal cell clones after lead poisoning and have found a marked depression in the femoral content of fibroblast-like (CFU-F) and adipocyte-like (CFU-FL) progenitors. We already have found that during this same time "stem cells" and "granulocyte progenitors" were elevated above normal. Clearly lead alters stromal cell proliferation *in vivo*. Similar measurements of CFU-F and CFU-FL in mice show a marked depression when erythropoiesis is stimulated and a large increase when erythropoiesis is suppressed. These results indicate that the stromal elements of hematopoietic tissue are based on the demand for hematopoietic cells. This concept is of considerable importance since evidence implicates these non-hematopoietic stromal cells in the regulation of the proliferation and differentiation of many hematopoietic cells. In our explorations of the above changes we noted that the requirement for exogenous hydrocortisone for stromal and hematopoietic growth could be eliminated if the cultures were grown in an O₂-poor atmosphere (5% CO₂, 5% O₂, 90% N₂) rather than the commonly used 5% CO₂-air environment. The nature of this changed steroid requirement is unknown, but our initial experiments suggest the involvement of some chemical released into the medium rather than a direct action of the low oxygen tension on all proliferating cells. The cells responding to the low O₂ pressure need to be characterized as does the substance involved. The low O₂ pressure corresponds quite closely to that expected in the marrow, suggesting that the hydrocortisone requirement at high O₂ pressure is not physiological. This finding is certainly a breakthrough and should provide a means for investigating the role of stromal cells in modulating hematopoiesis, especially "stem-cell" proliferation, in normal and pathophysiological conditions. The processes involved in regulating stromal cell activity both *in vitro* and *in vivo* forms the fundamental thrust of this proposed work.

(23) Manipulation of the Differentiated State by Oncogenesis
(k\$ 102)

R.I. Schwarz

Primary avian tendon (PAT) cells in a permissive cell culture environment will produce 48% of their total protein synthesis as procollagen. PAT cells malignantly transformed by Rous sarcoma virus will produce about $3.6 \pm 2.4\%$ procollagen. This drop in procollagen synthesis is accompanied by an approximately 14.4 ± 1.6 fold change in the level of procollagen mRNA. The major aim of this project over the next year is to elucidate the control steps that are altered after transformation that cause PAT cells to radically alter their commitment to procollagen production.

We will use a temperature-sensitive mutant in the *src* gene (LA 24) to study the kinetics of the transformation process as they relate to collagen expression. Specifically, PAT cells infected with LA 24 will be shifted from the nonpermissive temperature (41°C) to the permissive temperature (35.5°C), and changes in three critical steps in the collagen pathway will be analyzed over the next 24 h: levels of procollagen mRNA, rates of procollagen translations, and ability to secrete procollagen from the cell. Kinetically we will discriminate between the early rate-controlling steps that are directly sensitive to transformation and others that are secondarily controlled. Thereby, we plan to gain further insight into the mechanisms that regulate the differentiated state of PAT cells and insight into how these steps can be manipulated by malignant transformation.

(24) Endocrine Receptor Studies
(k\$ 210)

G.K. Clemons

The endocrine system is highly sensitive to a great variety of perturbations. We are using this sensitivity to find early indicators of hormonal alteration in animals exposed to environmental stresses to gain insight into the basic cellular and molecular mechanisms involved. Some of the effects of environmental stresses are transitory and reversible, and some are irreversible, especially in the young. The chemical stresses we are investigating are (1) ozone exposure and (2) nickel chloride administration. Superimposed low-level radiation will be used as a physical stress. The hormone systems we are mainly dealing with are the thyroid hormones, prolactin (PRL) and erythropoietin. The basic physiological phenomena in hormonal alteration caused by environmental perturbations will be pursued with a combination of radioimmunoassay, radioreceptor assay, and protein binding assays. This combination will enable us to study not only the specific actions of individual hormones but also the dependence and interaction with other hormones, especially in the developing young. The significance of this proposal lies in the need for sensitive early biological indicators of exposure to environmental stresses to assess the extent of possible harmful effects on man before irreversible pathological changes occur.

(25) Inducible Resistance to Alkylating Carcinogens
(k\$ 82)

R. Goth-Goldstein

In preliminary studies, I found that treatment of Chinese hamster ovary cells with toxic doses of some alkylating agents makes the surviving population permanently more resistant to the toxic effects of these agents. Resistance does not seem to occur by gene mutation or selection but rather by some other process.

I propose to define the process by which increased resistance is achieved in more detail. A resistant clone, which is representative of the resistant population and which has been stable in culture for 11 months, will be characterized with respect to its mutability by alkylating agents and its repair capacity. The frequency with which resistant clones occur at different treatment doses will be determined by use of a replica-plating method, and more clones will be tested in their response to alkylating agents to determine if they are equally resistant or if resistance increases with pretreatment dose. Also, more alkylating agents will be tested to determine which structural characteristics are necessary to increase resistance in progeny cells. Finally, it will be determined whether increased resistance after treatment with alkylating agents occurs in other cell lines and whether it depends on their initial sensitivity to alkylating agents.

The results will increase our understanding of how alkylating agents cause cell killing and what tolerance mechanisms are available to the mammalian cell to overcome the toxic effects of agents.

(26) Alkylating-Carcinogen: Mutagenesis in Mammalian Cells
(k\$ 95)

R. Goth-Goldstein

A variant of our Chinese hamster ovary cell line that is more resistant to the toxic effects of the alkylating carcinogen, MNNG, but equally mutable by it will be compared to the parent line in respect to sister chromatid exchange (SCE) induction by MNNG. This comparison will determine if SCE formation correlates with cell survival or with mutation induction.

A fluctuation test will be developed and used to determine whether the biphasic survival curve following treatment with methylating nitroso compounds is due to a resistant subpopulation or whether cell killing by these agents actually does not follow an exponential course. In addition this question will be investigated further by use of a replica-plating technique.

(27) Thymus-Marrow Interrelationships
(k\$ 175)

J.W. Goodman

The key to control of malignant growth and perhaps even the prevention of carcinogenesis lies in understanding the factors that play major roles in initiating and controlling cell division. It has been known for some time that thymus-dependent (T) lymphocytes (or T cells) and macrophages play such regulatory roles in the hematologic and immunologic systems. The mechanism(s) by which these cells exert their positive and negative controls over blood formation are of prime importance for reaching an understanding of regulation that will be of practical scientific and clinical use. Experimentally we first approached this subject by studying effects of lymphocytes administered to mice that had been irradiated and treated with bone marrow cells (i.e., to radiation chimeras). Very clear evidence that the two cell types interacted was obtained and published. To be able to control and observe more closely particular parameters of these cellular interactions, it was necessary also to use *in-vitro* methods, such as CFU-E, CFU-C, and BFU-E, that had been developed by others and that are standard assays currently in wide use in experimental hematology. Although it is conceivable that physical cell-cell contact can mediate the lymphocyte (or macrophage) effects on myelopoietic stem cells, it seems more likely to us that factors (called interleukins: e.g., IL-1, -2, -3) produced by the cells are responsible. Preliminary data from our studies confirm, for example, that IL-3 (purified to homogeneity) promotes survival of CFU-S, CFU-C, and BFU-E, in cultures. We propose to delineate a case in which a given interleukin produces a clear-cut effect on a particular cell lineage (e.g., erythroid) *in vitro* that mimics a result that has been seen in whole-animal studies. Specific anti-interleukin antibody will be used in attempts to abolish the effect *in vivo* and *in vitro*. Future work may also include purification and characterization of additional (as yet undefined) cell-derived factors. Results from these studies will contribute important information for the understanding of regulation and ultimately for the clinical control of abnormal cell division.

(28) Mechanism of Tumor Promotion
(k\$ 75)

M.J. Bissell

The major objective of this task is to understand the role of "oncogenes" in the context of differentiation, tumor promotion, and multistage carcinogenesis. An important conclusion that has emerged from the last fifty years of cancer research is that progression of cells from a normal phenotype to malignancy occurs in multiple stages. Until recently a major exception to this concept has been tumors induced by retroviruses, typified by Rous sarcoma virus (RSV). However, based on studies with temperature-sensitive mutant viruses, this laboratory proposed a few years ago that viral carcinogenesis might indeed involve both "initiating" and "promoting" events and that tumor promoters such as phorbol esters might act as promoters in virally "initiated" cells. Supporting evidence has since appeared from other laboratories as well as ours. In the last two years we have developed the capability of micro-injecting the viruses, or

tumor promoters, into the developing embryo. A startling observation has been that the wild-type virus, despite expressing its putative tumor-inducing gene product (pp60^{src}), is not oncogenic in the embryo. However, once the cells are disrupted and put in culture, they become rapidly transformed. Another exciting observation is that even in the newly hatched chick, RSV appears to be tumorigenic only when a wound is induced. A factor involved in wound healing, therefore, may be implicated in "tumor promotion." Techniques include using radioactive tracers, viral-specific antibodies and DNA probes, one- and two-dimensional SDS-PAGE, immunofluorescence, light microscopy, histological staining, and Southern and Northern blots. Future directions will involve probing the possible role of "endogenous oncogenes" in differentiation and malignancy, the reasons for the refractoriness of the early embryo to tumorigenic potential of RSV, and the role of wound healing in RSV tumorigenicity of the newly hatched chicks. The continued capability of probing transformation in culture and *in vivo* and the ability to micro-inject tumor viruses and tumor promoters into different sites should provide powerful tools for discovering the targets of oncogenes and for understanding the relation of transformation in culture to tumorigenicity *in vivo*. The system will also provide a versatile tool in basic studies of gene regulation.

(29) Molecular Carcinogenesis
(k\$ 395)

M.J. Bissell

That cancer is a problem of differentiation and gene expression has been appreciated for decades. Understanding what regulates gene expression at a cellular and molecular level, however, requires a rigorously defined and controlled environment. The general goal of the Laboratory of Cell Biology, and this task in particular, is a continued search for how to define "normal." This is a critical problem in its own right, but it is also an important approach in studying malignancy and disease. Cancer is most simply defined as the loss of normal regulation. By definition then, normal regulation has to be understood before one can understand the mechanism of such loss. That the basal lamina and the extracellular matrix (ECM) play a crucial role in maintenance of tissue specificity is becoming increasingly appreciated. The ECM is also known to influence the progression of malignancy and metastases. Our goal is to understand the molecular mechanisms of ECM-induced regulation and its loss after malignancy.

We have developed three interacting cell-ECM systems to study what we have referred to as "dynamic reciprocity." These include (1) mammary epithelial studies of "reversion" of tumor-virus-transformed cells on normal ECM. Common techniques include the use of electron microscopy, immunolocalization, monoclonal-antibody studies, cross-linking and inhibitor studies, two-dimensional SDS-PAGE of polypeptides, and, recently, the use of cloned genes for probing mRNA levels. We now can turn on and off many sets of functions and have embarked on a detailed analysis of how specific ECM components (including GAGs) are involved in tissue-specific protein synthesis and as signals in protein secretion and processing. Future directions will involve determination of routes of secretion of milk proteins as a function of changes in ECM components, cloning of normal genes expressed in culture and *in vivo*, identification of specific surface-cytoskeleton components involved in lumina formation, and an analysis of ECM components and how the ECM could influence the degree of transformation. The long-range implications of our studies encompass the regulation of milk production, assays for detection of preneoplastic lesions (by following changes in the patterns of differentiated products), a means of containing or reversing connective tissue tumors, and a more thorough understanding of factors that keep us healthy and functioning.

(30) Development of Metabolic Models for Alkaline Earth and Actinide Radionuclides
(k\$ 132)

P.W. Durbin

Metabolic models of the elements provide the biological components of radiation dose calculation schemes used to set protection standards for radionuclides and the framework for assessing the radionuclide content of the body from bioassay data. This project will compile, analyze, and report a large body of long-term metabolic *in-vivo* data developed for ^{90}Sr , ^{241}Am , and ^{238}Pu and use it to verify and/or modify metabolic models currently recommended by the International Commission on Radiological Protection (ICRP) for these radioelements.

Radiation protection standards limit the amount of radiation absorbed by workers and the general public and so serve as design guides for construction and operation of radiation and nuclear power facilities. The radiation dose limits used by the Nuclear Regulatory Commission (NRC) are those developed by the National Council on Radiation Protection (NCRP) and the ICRP. In the case of radionuclides, which may be deposited in the body, dose limits are met by limiting intakes, which in turn must be calculated using detailed numeric information for each element and its isotopes. The absorbed and deposited fractions and the time-dependent retention functions of the target tissues constitute the metabolic model for each element.

Isotopes of Sr, Pu, and Am dominate the potential long-term hazard of irradiated nuclear fuel and high-level fission wastes, and several of their isotopes and those of their chemical analogues are used in industry and medicine. This project contributes to the continuing improvement of the metabolic models for these important radionuclides. A unique aspect of this project is that it provides nearly continuous long-term blood and excretion data that can be used to improve assessment of radionuclide exposure from bioassay data.

(31) Biological Testing of New Actinide-Chelating Agents
(k\$ 57)

P.W. Durbin

The actinide elements (nearly all are alpha emitters) are carcinogenic if deposited and retained in bone, lung, or liver. They are poorly excreted and largely recirculated and redeposited; the only way known to reduce the radiation risk is to accelerate their excretion with chelating agents. Potent, selective iron-sequestering agents produced by microorganisms contain weakly acidic functional groups—catechol in enterobactin and hydroxamate in the ferrioxamines. The similar chemical and circulatory transport properties of Pu(IV) and Fe(III) suggested that macromolecules containing those electron-donor groups would chelate Pu(IV) at pH 7 and not bind essential divalent metals. Macromolecules have been prepared containing catechoylamide (CAM), hydroxamate (DFO), and/or hydroxypyridinone (HOPOCAM) groups connected by alkyl chains. The potency of those ligands for promoting Pu(IV) excretion has been demonstrated. The most effective ligands are straight-chain structures containing three or four functional groups acidified with a sulfonate CAMS or carboxylate CAMC substituent on the benzene rings; their hydrophilicity can be controlled, their excretory route shifted to feces, their biological retention prolonged by adding alkyl groups to the terminal N's. All ligands are tested for acute toxicity. Less hydrophilic ligands are tested for delayed Pu excretion (7 days). Prototype ligands are (or will be) tested for dosage effectiveness and the efficacy of extended multiple ligand injections. Planned research includes: screening new ligands for Pu removal and acute toxicity; completing the above tests and obtaining descriptions of the biokinetics for the prototypes, 3,4,3-LICAM(C), desferriCAM(C), and 3,4-HOPOCAM; conducting special studies, e.g., stop-flow preparation to investigate renal tubular secretion of the hydrophilic, sulfonated CAM ligands; developing a test of oral ligand activity; and developing an *in-vitro* test of ligand toxicity using cultured C3HT101/2 (mouse embryo) cells to supplement *in-vivo* toxicity screening.

(32) Quantitative Species Extrapolation in Carcinogenesis
(k\$ 298)

B.N. Ames

We will use a comprehensive data base to address several issues relevant to the use of animal bioassay data in estimates of carcinogenic risk to humans.

1. How replicable are the results of animal cancer tests?

There are many chemicals in the literature that have been tested twice in the same sex of the same strain and species using the same route of administration. We will investigate the extent of replication in terms of three experimental outcomes: (a) evidence of tumorigenicity (hereafter positivity); (b) carcinogenic potency (TD_{50}); and (c) target sites. We have begun to examine this question with the chemicals included in the National Cancer Institute (NCI) Bioassay Program. Among 47 experiments on ten chemicals in rats and 31 experiments on six chemicals in mice, there is consistent evidence of reproducibility of results for positivity, potency, and target organs. This replication occurs in spite of differences in the length of dosing, dose levels, and number of dose groups. We will use all such cases on all chemicals in a data base to examine the issue of reproducibility *in vivo* of results.

2. How well do experiments in one species predict the results of experiments in a second species?

All of the NCI chemicals and many other chemicals as well have been tested in more than one species. We will use such experiments to investigate the same three outcome measures: positivity, potency, and target organs.

We have found very high correlations between the potencies of rats and mice in our analyses of the NCI bioassays and are currently examining the reasons for this correlation. We will describe which chemicals induce tumors at a particular site for each species and the range of carcinogenic potency of chemicals that induce tumors at a particular site. In addition we will investigate whether chemicals that induce tumors at a given site are likely to be positive in a second species and/or at another site in the same species.

(33) Genetic Effects of Carcinogens in Mitosis and Meiosis
(k\$ 128)

M.S. Esposito

The yeast *Saccharomyces cerevisiae* provides a model eukaryotic system with which to assess the genetic effects of physical and chemical carcinogenic agents during mitosis and meiosis. Our previous studies of the mechanisms of spontaneous mitotic and meiotic recombination have led to the development of genetic techniques that we employ in the present experimental program to characterize the effects of x rays, ultraviolet light, ethyl methanesulfonate, and ethylnitrosourea on gene mutation, intragenic recombination, intergenic recombination, and chromosomal nondisjunction and/or loss following exposure of diploid hybrids to these agents during mitosis and meiosis. Synchronous mitotic and meiotic populations will be employed to determine whether these agents exert their genetic effects at discrete times during mitosis and meiosis. The mitotic studies proposed employ *MATaMATa* hybrids and congenic *MATaMATa* and *MATaMATa* strains. The use of diploids homozygous at *MAT* facilitates the genetic analysis of putative nondisjunctions. The analysis of meiotic populations focuses upon full genetic characterization of the various cell types present following exposure of sporulating cultures to mutagen-recombinogens, including mitotic diploid cells, meiotic diploid cells, and ascospores. We anticipate that a comparative study of this type will contribute to further understanding of the mechanisms of mitotic-versus-meiotic induced mutation, recombination,

and chromosomal nondisjunction.

(34) Inducible Responses to Carcinogenic DNA Damage
(k\$ 169)

P.K. Cooper

Our broad objective is to understand inducible cellular responses to DNA damage by carcinogens, many of which are mutagens in bacteria, with special emphasis on understanding the relationship between those responses that contribute to cellular survival following carcinogenic damage and those that affect mutagenesis. We use *E. coli* as a model cell system in which to study inducible SOS responses and adaptive responses, evidence for both of which has also been found in mammalian cells, because of the advantage of availability of relevant mutants and extensive biochemical and genetic characterization. Immediate research objectives include:

1. *Factors involved in inducible repair of UV damage and characterization of its mechanism.* Having shown that the primary process resulting in enhanced cellular survival and Weigle reactivation by SOS induction is *uvr⁺* dependent and correlates with long-patch repair, we are attempting to determine which induced gene products are required and in what capacity. We are also investigating the detailed mechanism of the process to determine whether lesion removal is involved or whether an incision-initiated event that contributes to tolerance of persistent damage is responsible.
2. *Substrate for long-patch repair of UV damage.* Having obtained evidence suggesting that long patches occur at some particular small class of damage sites that are refractory to constitutive repair and that are apparently potent blocks to replication, we are investigating the nature of these sites as an approach to understanding the means by which the inducible process contributes to survival. We are particularly interested in the possibility that lesions in some functionally distinct region of the genome, perhaps growing point regions, are involved.
3. *Inducible repair of alkylation damage.* Having found that inducible repair synthesis occurs after MNNG damage as it does after UV, we are exploring the extent to which this represents an overlap between the two known inducible processes, the SOS and the adaptive responses, and the means by which it contributes to survival of alkylation damage.

(35) Carcinogenesis and Life Span Studies
(k\$ 355)

E.J. Ainsworth

This continuing research program is directed toward the elucidation of the interactions between high-energy multi-charged ions (heavy ions) and biological materials for assessment of the life-shortening and carcinogenic hazard of cosmic particles to man in space.

Cellular Studies. The range of heavy-charged-particle LET's (linear energy transfer) studied so far is from 10-190 keV/ μ m. Results show the relative biological effectiveness (RBE) for neoplastic transformation increases with LET, and RBE is inversely related to dose. During the coming year studies with ^{56}Fe will be continued. Studies with selected heavier ions will be initiated to determine the RBE at an LET greater than 190 keV/ μ m. Definition of the LET range over which the RBE for neoplastic transformation remains high is important for risk assessment and is also of fundamental biophysical interest. Additionally, because of the potential importance of synergisms between low- and high-LET radiation, experiments on neoplastic transformation under these conditions were initiated last year. Possible synergistic effects have been demonstrated. During the coming year such effects will continue to be examined using high-LET ^{28}Si or ^{40}Ar ions and 225 kVp x rays. Mutagenesis studies with the mammalian cells (C3H10T1/2 SV) cultured *in vitro* using 6-thioguanine resistance as the genetic marker will be continued to evaluate RBE-LET relationships. Results from this study indicate high mutagenic

effects of ^{28}Si ions, and during FY 1985 studies with ^{40}Ar and ^{56}Fe particles will be initiated.

Life Span Studies. Results indicate that the life-shortening effects of ^{12}C are appreciably less than those of fission-spectrum neutrons, which are characterized by a similar LET, and that fractionation of ^{12}C doses produces little or no sparing effect on life shortening. In contrast, fractionation of ^{60}Co gamma radiation produces a marked sparing effect. Life span studies on exposure to single doses of heavier charged particles have not yet progressed sufficiently for preliminary conclusions to be drawn. In FY 1985 LBL will continue monitoring life spans and tumor prevalence and will initiate studies with 24 fractions of ^{20}Ne ions.

(36) Long-Term Biological Effects
(k\$ 255)

E.L. Alpen

Objective. The continuing objective of this program is to determine and assess the importance of the acute, chronic, and long-term effects of high-LET (linear energy transfer) radiation on normal tissues. We will also evaluate the LET dependence of the carcinogenic potential of charged particles and examine the shape of the dose-response relationship at low doses.

Approach. The organ systems that will be studied are the kidney, the gastrointestinal system, bone marrow, lung, and spinal cord. The Harderian gland system will be used to assess radiation carcinogenesis. Single-dose responses will be investigated for these various systems in addition to fractionation schemes that allow analysis of repair and recovery. These studies will be conducted in the plateau region of heavy-ion beams for clarification of RBE with respect to LET, ion mass, ion charge, and track structure.

Accomplishments. Preliminary results from experiments with heavy ions suggest that the RBE-to-LET relationships for cancer induction in the Harderian gland does not show a marked peak at 100 keV/ μm as seen for some other endpoints. Preliminary heavy-ion gut-repair studies have been conducted, and there appears to be some recovery but not to the extent that occurs after low-LET irradiation. Pulmonary studies indicate a late (36 weeks) fibrotic-induced increase in respiratory rate. The single-dose acute studies in bone marrow, gut, and spheroids indicate that the LET for maximum RBE is about 100 keV/ μm . The LET value is lower than the LET for maximum RBE in *in-vitro* monolayer cells.

Expected Accomplishments. We will continue to assess the carcinogenic potential of heavy ions in the Harderian gland system. Characterization of chronic and late effects of single and fractionated doses of heavy-ion irradiation on kidney and lung function will be emphasized. Studies on normal tissue and spheroids will clarify the RBE with respect to LET.

Implication of Accomplishments. Studies to date indicate that organized tissues have a different LET dependence than that found for cells *in vitro*. We are evaluating the fundamental differences between the repair processes of organized tissue and those for single cells in culture. These data have direct application for medical use of heavy charged particles and for estimating the potential hazards of cosmic radiation in the space environment.

(37) Effects of Heavy-Particle Radiation
(k\$ 410)

J.I. Fabrikant

Objective. To apply narrow beams of accelerated heavy ions (*viz.*, He, C, Ne) to the mammalian brain to examine CNS cellular response and cell population kinetics, regulatory control mechanisms, and homeostasis, including myelinogenesis and cerebral blood flow dynamics.

Rationale. The physical and biological properties of narrow heavy-ion Bragg-peak beams provide neuroscience probes for investigating biochemical and physiological effects in the mammalian brain: tissue injury and repair and the dependency upon dose, dose rate, volume, and

time of the induction of CNS damage at various sites.

Experimental Approach. Biophysical studies to investigate heavy-ion beam quality and RBE/LET relationships of cell and tissue injury in mammalian brain; neurochemical and metabolic probes to examine cellular response, nucleic acid metabolism, cell proliferation kinetics, and myelinogenesis; radioisotope-labeled nucleic acid and cerebroside precursors to tag newly formed cells. In addition, biochemical moieties and their fates are traced with high-resolution autoradiography; NMR and SPECT image brain tissue response and cerebral blood flow following heavy-ion irradiation in rodents and humans are investigated.

Progress. Research examines physical and biological properties of narrow heavy-ion beams at 184-Inch Synchrocyclotron and Bevalac; nucleic acid metabolism, cellular response, and cell population kinetics in irradiated mammalian brain; quantitative NMR and SPECT imaging of radiation injury and repair in brain.

Significance. To gain a better understanding of response of various brain cell populations following induction of discrete CNS lesions with narrow heavy-ion beams in various neuroanatomical sites; to elucidate neurophysiological and neuropathological responses, radiation injury and repair, in mammalian brain; to apply heavy-ion radiosurgery; to study and treat human brain disorders.

Future Directions. Elucidation of biochemical anatomy and temporal patterns of mammalian brain cell and tissue response to cerebral irradiation with heavy-ion beams at the Bevalac; mechanisms of regulatory control and homeostasis of brain-cell proliferation and differentiation kinetics, myelinogenesis and cerebral blood flow using radioisotope and NMR techniques; applications of heavy-ion Bragg-peak beams at the Bevalac for study of human brain response and treatment of CNS disease.

(38) Radiological Physics and Chemistry (k\$ 334)

A. Chatterjee

The subject of this project is physical and chemical changes in biomolecules caused by radiation injury. Our goal is to understand the mechanism of biological damage (to mammalian cells) caused by radiation exposure. Such an understanding must develop from the fundamental principles of physical, chemical, and biological laws.

Through an understanding of the detailed mechanism (as much as possible) of the damaging effects of radiation on organisms, we may learn how to use radiation most effectively in the diagnosis and treatment of disease and how to provide effective protection against the occupational and environmental hazards of radiation.

Initially, the experimental approach involves relatively simple biomolecular systems such as aqueous solutions of ϕ X-174 DNA and SV40 viral DNA and various qualities of ionizing radiation. Following the investigation of these systems and protein solutions (next in line), highly complex mammalian cell systems will be studied. In each experimental system, results will be analyzed in terms of theoretical models. Results in the ϕ X-174 and SV40 systems are obtained as single- and double-strand breaks as experimental endpoints. Such endpoints have direct relevance to damage in the mammalian cell systems. To determine the extent of damage for a given type of radiation, quantitative information will be obtained by analyzing the single- and double-strand breaks in a Varian spectrophotometer and a gel scanner. Results can be obtained almost immediately following irradiation. The types of radiation to be used are x-rays, ^{60}Co - γ rays, and particulate α rays.

The quantitative information on the extent of single- and double-strand breaks in ϕ X-174 DNA solutions is already available for x rays and ^{60}Co - γ rays. Theoretical analyses of these

results connecting the physical, chemical, and biological stages are in progress.

As progress is made toward achieving the objective, we will have better control of radiation as an environmental hazard and as a medical tool, particularly in cancer diagnosis and therapy. Once the objective is achieved, efforts will be made to study specific chemicals and their protective properties against radiation damage.

(39) Measurement of the Production of Neutrons by High-Energy Heavy Ions
(k\$ 60)

W. Schimmerling

This research program consists of integral experiments to measure fluence spectra of nuclear interaction products caused by relativistic heavy-ion beams from the Bevalac accelerator system incident upon thick targets related to atmospheric, tissue, and spacecraft constituents. The results will provide knowledge, not otherwise available, of importance in evaluating the radiation environment of long-term space missions, e.g., large space structures and the Space Operations Center systems presently being considered for low-earth-orbital missions. Specifically, we will:

1. Measure the velocity, charge, and (where possible) mass of all particles emerging from thick targets of carbon, aluminum, silicon, iron, and lead, as well as some selected plastics such as graphite-epoxy, for relativistic heavy-ion beams of He, C, Ne, A, Fe, and U (or Pd), incident at energies between 200 and 2000 MeV per nucleon and for target thicknesses comparable to the particle ranges, at 0° to the beam.
2. Repeat the above measurements to obtain the angular distribution of emerging particles.
3. Use these results, with computer codes under development, to predict the transport of relativistic heavy ions in configurations of interest to space applications.

(40) Response of Tumor Cells to Heavy Ions
(k\$ 284)

S.B. Curtis

The objective of this research is to study the response of a well-characterized tumor system (presently the R-1 sarcoma in the WAG/Rij rat) to heavy charged-particle radiation from the Bevalac.

The studies are designed to provide information on the importance of cellular processes such as repopulation, variations in cell kinetic parameters, and possible interactions of lesions produced by high- and low-LET radiation in affecting tumor response *in vivo*. Specifically, these studies will (1) measure the repopulation kinetics of the surviving cell population after either heavy charged-particle or X-irradiation; (2) measure post-irradiation cell kinetic parameters by flow cytometric techniques for both the entire population and the surviving population only, using a fluorescent DNA stain of low toxicity (Hoechst 33342)—cells in the various cell-cycle phases will be sorted on the basis of DNA content and used for measurements of phase-specific cell survival; (3) determine if there is a measurable interaction between unrepaired lesions produced by heavy charged-particle radiation and subsequent X-irradiation *in vivo*; and (4) continue the development of a model of tumor response incorporating the data obtained.

(41) Heavy-Ion Radiobiology Related to Oncology
(k\$ 1,082)

C.A. Tobias

The aim of this program is to furnish a quantitative framework for the effective use of heavy accelerated particles in therapeutic investigations at the Bevalac. Heavy-ion beams have biologically effective depth-dose distributions and a low oxygen effect that are efficacious for the treatment of hypoxic tumor cells. Heavy ions also reduce the differences in radiosensitivity during the cell division cycle and the extent of repair of radiation damage. Of particular interest are high-energy silicon and neon beams with a therapeutically useful depth of penetration (~25 cm). On the basis of current radiobiological information, these elements appear to have advantages over both lighter and heavier elements in terms of simultaneously achieving a high biologically effective dose and a low OER in the tumor treatment zone. The cellular radiobiology project will use synchronized human cells in culture to analyze the mechanisms underlying the production of heavy-ion lesions, the magnitude of the oxygen effect, the repair of sublethal and potentially lethal damage, and the potentiation of injury that occurs in fractionated dose schedules with very high-LET radiation. The heavy-ion radiobiology of sensitive and resistant cell lines will also be studied. The degree of heavy-ion-induced molecular injury in DNA will be quantified and related to cell survival. The normal tissue radiobiology program is focused on the effect of single and protracted heavy-ion exposures on certain critical organs such as gut, lung, spinal cord, and brain. The oxygen effect will be studied *in vivo* in testes. Brain radiation injury will be assessed by nuclear medicine techniques. Special instrumentation is being developed in the pretherapy physics program to rapidly quantify beam fragmentation spectra. A repair-misrepair hypothesis is being used to model bioexperiments and to predict the results of protracted dose schedules. The core project carries out applied radiobiology experiments in support of patient therapy.

(42) Molecular Mechanisms of Cellular Effects
(k\$ 180)

C.A. Tobias

Our effort is directed toward a basic understanding of the molecular lesions and the cellular kinetics of biological responses to accelerated beams of heavy nuclei. The Bevalac is a unique source of these beams, and the heavy-ion program is of interest not only to DOE but also to the National Cancer Institute (NCI) and the National Aeronautics and Space Administration (NASA). The results obtained and models developed to explain and quantitate our observations will not only provide an essential foundation for the use of heavy ions in the diagnosis and treatment of disease, but also may be of value to the understanding of radiation hazards of high-LET radiations in interplanetary space and at nuclear reactors. We experimentally separate the events that cause the formation of lesions along heavy-ion tracks in the DNA of mammalian cells from the biochemical repair responses and genetic consequences. We find that among the important heavy-ion-induced lesions is the DNA double-strand scission. We also demonstrated that cultured mammalian cells can repair most of these double-strand breaks by enzymatically rejoining the strands. A quantitative model developed here (the Repair-Misrepair Model) assumes that two kinds of repair exist: curepair is a process that permits resynthesis of the genetic material and rejoining of the strands so that its coding will be indistinguishable from normal; misrepair incorrectly joins DNA strands together. We believe that the misrepair process is responsible for lethal effects and for mutations involving gross DNA rearrangements. Studies with ataxia telangiectasia cells have indicated that their radiosensitivity may be the result of misrepair of the radiation-induced lesions. We have shown that oncogenic transformation by viruses is greatly enhanced by heavy-ion irradiation. We constructed plasmids containing an oncogene (gene A of the SV40 virus). By the process of transfection, we demonstrated that radiation will enhance the integration of genetic material into the DNA of host mammalian cells. The integration process can also be classified as misrepair. In the future, we wish to clarify the molecular and enzymatic processes involved in misrepair.

(43) Physical Characteristics of Heavy-Ion Beams
(k\$ 200)

W. Schimmerling

Heavy-ion beams stopping in tissue consist of primary particles and fragments caused by nuclear interactions in the materials presented to the beam. These fragments are a significant component of the dose, especially near the Bragg peak and distal volume. Conventional dosimetry does not identify the fluence, charge, and velocity of these components. Biological effects (e.g., RBE and OER) depend on these quantities rather than on mean LET alone. An understanding of this dependence in terms of a chemical theory of track structure likewise requires a knowledge of these dose components. The present research will provide a complete characterization of heavy-ion beams at the Bevalac by particle identification and direct measurements of fluence and velocity. This is accomplished with a multidetector particle-identification spectrometer consisting of a time-of-flight telescope, pulse ionization chambers, and a 10-element silicon detector telescope, as well as scintillation counters and multiwire proportional chambers for beam definition. The apparatus is being used initially to identify nuclear reaction products and primary beam particles emerging along the central axis of the beam from a water absorber, as a function of absorber thickness. Unmodified beams of carbon, neon, silicon, and argon are being studied in an especially designed beam line. Studies of ridge-filter-modified beams and off-axis measurements will follow. Chemical dosimetry and radiobiological experiments will be performed to establish the parameters governing beam equivalence with the BioMed facility. Beam transport calculations are being developed to obtain a reliable beam model for extension of the results to arbitrary configurations. The use of the completely characterized radiation fields for experiments in radiation chemistry and radiobiology will result in a better understanding of the fundamental mechanisms of radiation action. The results of this research will be incorporated into treatment planning for clinical trials of radiation therapy currently in progress at the Bevalac.

(44) Treatment of Cancer with Heavy Charged Particles
(k\$ 2,179)

J.R. Castro

This research project will study the therapeutic application of heavy charged particles such as helium, neon, or silicon ions in the treatment of human cancers to test the potential advantages of improved dose distribution (helium) and increased biological effect (neon, silicon). Continued refinement of fractionated, large-field, spread-out-Bragg-peak charged-particle radiotherapy treatment techniques is being sought together with improvement of techniques for assessment and compensation of tissue inhomogeneities using CT and NMR scanning in treatment planning.

Current pilot studies with neon and silicon ions will lead to prospective controlled clinical trials. Our ultimate goal is to test heavy charged particles against the best available therapy in a randomized trial of selected tumors. Existing cooperative study groups such as the Radiation Therapy Oncology Group and the Northern California Oncology Group are used to facilitate these trials, together with the Bay Area Heavy-Ion Association.

(45) Charged-Particle-Beam Dosimetry Task Group
(k\$ 29)

J.T. Lyman

This is a project to identify and find solutions to those problems in basic physics, dosimetry, and clinical applications associated with the use of charged-particle beams in the treatment of human cancer. This will be accomplished by collaborative efforts among physicists in the American Association of Physicists in Medicine who are actively working on projects where patients are already being treated with charged-particle beams or where serious efforts are under way to develop such projects. Particular attention will be given to those investigations that will provide techniques, data, and information that solve problems common

to all charged-particle therapy facilities, regardless of the particle employed, and for which funding is not available through other institutional grants.

Charged-particle therapy is in a period of rapid development. As in any new field, there are problems, many of which are common to all of the projects regardless of which particle is employed. This task group will ensure the compatibility of dosimetry practices at all facilities and will enable earlier and more efficient solutions to be found to pressing problems.

An important result of this work will be the development of a charged-particle-beam dosimetry protocol that will serve as a standardizing document for all charged-particle-beam therapy facilities and as a guide to agencies that may oversee the quality control of charged-particle-beam clinical trials.

(46) Evaluation of Treatment Planning for Particle Beam Radiotherapy
(k\$ 72)

J.T. Lyman

The primary goals of this program are the following:

1. To develop treatment plans for selected patients with tumors in the major anatomic sites to be treated with helium and heavier charged-particle beams.
2. To establish in patients and in phantoms that the desired treatment plans can be accomplished.
3. To calculate a biologically equivalent dose treatment plan for these patients.
4. To verify in phantoms that the dose distributions do produce the anticipated biological response.
5. To make necessary dosimetry and microdosimetry measurements to characterize the helium and heavier-ion beams.
6. To help in defining RBE's for normal tissues and maximum allowable doses to critical organs for each particle beam.
7. To help in defining standard procedures for dosimetry and microdosimetry measurements in patients and phantoms.
8. To help in defining common criteria for calculating biologically equivalent doses.
9. To help in defining common criteria for tissue density inhomogeneity corrections.
10. To participate in the evaluation of treatment plans and the corresponding *in-vivo* and phantom measurements for each anatomic site and each particle beam and to assess the effectiveness of delivering the prescribed total and biologically equivalent dose to the treatment volume by each particle beam system.
11. To participate in the comparison of the treatment plans and the corresponding *in-vivo* and phantom measurements to assess the relative effectiveness of each particle beam for the treatment of tumors in each major anatomic site.
12. To participate in the comparison of the treatment plans and the corresponding *in-vivo* and phantom measurements to assess the relative effectiveness of each particle beam for the treatment of tumors in each major anatomic site.

(47) Tracer Studies with Radioactive Beams
(k\$ 75)

A. Chatterjee

This project involves development of a technique to concentrate radiation dose on a tumor volume while sparing surrounding normal cells and nearby critical organs.

Some cancer patients are undergoing therapeutic treatment with particulate radiation instead of ^{60}Co gamma radiation or x rays. With particulate radiation it is possible to concentrate radiation dose mostly in the tumor volume. The objective of this project is to devise a practical method to concentrate, on a routine basis, the radiation dose on the desired target with a reasonable degree of accuracy.

Among the various modalities of treating cancer patients, radiation therapy provides an important means of controlling the disease. Hence, efforts should be made to deliver this modality in the best possible manner, to derive its maximum benefit.

The experimental approach consists of using radioactive particles such as neon-19 or carbon-11. Both of these particles decay by emitting positrons, which then annihilate with the medium electrons to produce two gamma rays, separated by 180° . These gamma rays can then be detected in coincidence mode by a positron camera (already available) to locate the stopping point of the beam. Through proper adjustment of the energy of the beam, the stopping point can be controlled to coincide with the tumor volume. Since radioactive beams and therapeutic beams are similar, our objective can be achieved through this approach.

High-intensity radioactive beams of both neon-19 and carbon-11 have been produced, and on-line tests have been performed. It has been demonstrated that using this technique, radiation dose can be concentrated on a desired target volume.

By this technique, great progress will be made toward delivering radiation treatment to cancer patients under optimal conditions. The success rate of the treatment will be greatly enhanced, and many patients will derive benefits.

In the immediate future, in a few selected patients, this technique will be applied and the results will be evaluated for routine treatment planning.

(48) Heavy-Ion Radiosurgery
(k\$ 290)

J.I. Fabrikant

Objective. To establish stereotactic heavy-ion Bragg-peak radiosurgery for brain disorders, including intracranial arteriovenous malformations (AVMs), as a nuclear medicine research method applied to the study of brain disease in man and to examine physical and biological properties of stereotactically directed narrow heavy-ion beams in the CNS, for improving methods of dose-delivery and dose-distribution and for establishing RBE/LET relationships for CNS tissue response.

Rationale. Narrow beams of helium ions have superior biological and physical effects in the brain over x- and gamma rays; heavy ions at the Bevalac have advantages over helium ions and protons for CNS disorders in man, including less range straggling and multiple scattering for same residual range in tissues, improved dose distribution in Bragg peak, and sharp lateral and distal borders, with greater sparing of critical adjacent CNS structures.

Experimental Approach. Interactive charged-particle treatment planning and instrumentation/engineering design allow delivery of narrow heavy-ion beams to predetermined, three-dimensional target volumes within brain or spinal cord; quantitative NMR and SPECT imaging at UCSF.

Progress. In the clinical research program over 55 radiosurgical brain patients with intracranial vascular disorders have been studied and treated with charged-particle beams. Research activities have expanded to applications of NMR and radionuclide SPECT imaging of CNS tissues treated with heavy ions.

Significance. On the average, 500,000 people in the United States have life-threatening AVMs; the annual rate of rupture is 2-3%; and the rate of rebleeding is 6% in the first year after hemorrhage and 2%/yr thereafter. About 10% die with first hemorrhage, 20% with each rebleeding. Stereotactic heavy-ion Bragg-peak radiosurgery has the potential of conferring protection against rebleeding, in many cases leading to obliteration of the lesion with minimal morbidity and no mortality.

Future Directions. The work will include: continued modifications and improvements of radiosurgical method to establish the long-term benefit of treatment of brain with stereotactically directed narrow beams of accelerated charged particles; quantitation, using NMR and SPECT, of CNS tissue injury and repair and cerebral blood flow alterations following cerebral heavy-ion irradiation; and development of the method of stereotactic heavy-ion Bragg-peak cerebral irradiation (carbon and neon) at the Bevalac.

(49) Experimental Medicine Development (k\$ 220)

Y. Yano

The objective is to develop methods for the production of radioisotopes and for the labeling of biochemical substrates to investigate human physiology and metabolism by noninvasive procedures using emission computed tomography (ECT).

Radiolabeled biochemical substrates follow the same metabolic and blood flow pathways as naturally occurring material; thus it is possible to quantitate moment-to-moment changes in concentration of the radiotracer to compare turnover and uptake in normals compared to diseased states.

The approach is to develop radioisotope generators (the most economical and readily available source of short-lived radioisotopes) and the cyclotron production of the radioisotopes of carbon, nitrogen, oxygen, and the halogens for incorporation into biochemical compounds. Generator development includes studies of the nuclear-accelerator or -reactor production of the long-lived parent radioisotope, the ion-exchange properties of organic and inorganic adsorbents, and elution parameters with physiologically compatible solutions.

Cyclotron production involves target development to meet the requirements of high pressure, high temperature, remote operation of gas flow targets, high chemical and isotopic purity of target materials, and radiochemical and radionuclidic analysis. Labeling chemistry requires development of rapid and remotely controlled organic and enzymatic syntheses.

Progress has been made in providing multi-millicurie amounts of amino acids, fatty acids, sugar analogues, and H_2O labeled with carbon-11, nitrogen-13, oxygen-15, and fluorine-18 for ECT studies of flow and metabolism. Generator-produced rubidium-82 has been available for studies of myocardial blood flow and blood brain barrier permeability. Generator-produced gallium-68 has been used to label platelets, proteins, and lipoproteins to study thrombosis and atherosclerosis.

The significance of these developments is that many biochemical substrates and antagonists for specific receptor sites can be radiolabeled to study metabolism and receptor-site binding alterations in various brain diseases. Cardiovascular disease can be diagnosed and studied with radiolabeled platelets, lipoproteins, and monoclonal antibodies. The latter is also applicable to tumor diagnosis and therapy.

(50) Scatter Compensation in Emission Tomography
(k\$ 115)

R.H. Huesman

Scattered photons, which carry false information and make a large contribution to noise in emission tomography, can constitute as much as 50% of the total events collected depending on the construction of the imaging instrument. This contribution is not uniform in the majority of situations and will necessarily lead to erroneous interpretation of data when quantitative results are sought. Whereas some simple computational schemes have provided methods for removing the majority of scatter background in positron-emission tomographs for head imaging, these methods are not applicable to the general problem of variable attenuation coefficient nor to recent tomographic designs that seek to minimize interplane shielding to collect coincidence data, within a greater solid angle. Neither do existing methods compensate for off-plane sources such as spleen and liver activity which can contribute serious data distortion in transverse-section imaging of the thorax.

We propose to remove the scatter contribution and to optimize design of single-photon-emission and positron-emission tomographic shielding and detector configurations. Our methods rely on rigorous Monte Carlo simulations that use the Klein-Nishina collision cross sections in a flexible computing architecture. An essential tool developed for this application allows for variable attenuation and tracks the trajectories of photons in three dimensions. Through the use of these Monte Carlo methods the scatter background will be characterized for general cases of distributed sources and scattering media.

The expected benefits of this research are twofold: first, an efficient algorithm will be developed for removal of in-plane and off-plane scatter contributions by iterative schemes or deconvolution methods; second, the results of these calculations will be used to examine various shielding and detector configurations for improved quantitation in high-resolution positron tomography with multilayered tomographic designs.

(51) Bragg-Peak Localization by Radioactive Beams
(k\$ 338)

A. Chatterjee

The Bragg-peak therapy of cancer patients with heavy charged particles requires precise localization of the Bragg peak in a tumor volume. A slight error can cause severe underdosing of the tumor region and overdosing of nearby critical organs.

For precise localization of the Bragg peak, one requires an experimentally measured value of the water equivalent thickness between the point of entry and the target volume. Between these two end points there can be unknown amounts of bone, tissue, sinus, air, etc.

Presently used cancer therapy techniques may not be as reliable as desired, especially when there is a large amount of thick bone or long air path. We have developed a technique that uses a high-energy radioactive beam and a sensitive positron camera and that, we expect, will achieve the desired accuracy.

In this technique, radioactive particles such as ^{19}Ne or ^{11}C are used. Both of these particles decay by emitting positrons, which then annihilate with the medium electrons to produce two gamma rays, separated by 180° . These gamma rays can then be detected in coincidence mode by a positron camera to locate their origin in space.

Through adjustment of the energy of the radioactive particles (mostly ^{19}Ne will be used), they will be stopped on the location of the tumor, as verified by the positron camera. This method provides a direct measure of the required water equivalent thickness. This technique will be applied in the treatment position (on line) and just before the actual therapy. Unlike x rays (used in cancer therapy), radioactive particles have penetration properties that are very

similar to those of the heavy charged particles used in Bragg-peak therapy. The value of the water equivalent thickness measured by a radioactive beam is then directly applicable for treatment planning with heavy charged particles. Precise delivery of Bragg-peak dose on a tumor volume, while sparing the normal cells and nearby critical organs, constitutes an extremely important component of the evaluation of heavy-particle treatment modality. This is a long-term goal of the laboratory.

(52) Cardiovascular Flow and Metabolism
(k\$ 805)

T.F. Budinger

The two major themes of this project are: (1) the development of methods for evaluation of myocardial flow and metabolism in man using positron emission tomography (PET) and nuclear magnetic resonance (NMR); (2) the investigation of the biological and biochemical behavior of the arterial wall in man and animals using noninvasive methods of high-resolution PET and NMR. The program is divided into 5 projects and two cores. *Project 1* is devoted to early detection of myocardial ischemia using PET imaging of F-18-2-deoxyglucose and Rb-82 and to investigations of the distribution and kinetics of methionine and taurine in the myocardium. A major question is the evaluation of cation transport under conditions of reperfusion in the compromised myocardium. *Project 2* focuses on ischemic brain disease and the efficacy of hyperbaric oxygenation and fluorocarbons, using autoradiography in the CAT model and PET with 1-122-phenylalkylamine as a new cerebral blood flow method. *Project 3* is devoted to a comparison of PET to NMR for the detection of ischemic heart disease. Measurements of the NMR characteristics of carotid and aortic atherosclerotic plaques by *in-vitro* and *in-vivo* approaches are planned. NMR health hazards for the ischemic heart and embryogenesis caused by rapid field changes will be studied. An NMR evaluation of endogenous C-13 spectra of skeletal muscle at various stages of exercise and in patients with abnormal serum lipoprotein patterns is also proposed. *Project 4* is an instrumentation development project for a PET with 2-3 mm spatial resolution. New detector methodologies are to be developed for a multilayer high-resolution system to be used in labeled platelet and lipoprotein studies of the PPG. *Project 5* proposes new methods for data acquisition from multicrystal PET devices for the reduction of PET data to physiologically meaningful parameters. Expected goals are completion of a practical protocol for PET clinical studies of myocardial ischemia; development and application of practical techniques for evaluation of platelet dynamics *in vivo*; development of a method for imaging the composition of aortic plaques *in vivo*; new knowledge regarding the kinetics of lipoprotein subclasses; and new knowledge regarding lipid and glycogen turnover in skeletal muscle.

(53) Positron Three-Dimensional Imaging Instrument
(k\$ 205)

S.E. Derenzo

The objective of this project is the development of advanced detector concepts for the *imaging of positron-labeled tracers in man and animals* with substantial improvements in spatial and temporal resolution. Our tomograph design approach is to encircle the patient with rings of small, close-packed, bismuth germanate (BGO) scintillation crystals individually coupled to photosensors.

An ultrahigh-resolution positron tomograph presently under construction consists of a single ring of 600 BGO crystals 3 mm wide and will be used in associated medical research projects for studies of the human brain and for heart and brain studies in animals. Using sub-optimal opposing arrays of such crystals in a special computer-controlled test gantry, preliminary measurements show a circular point-spread function (PSF) at the center of the gantry with a full width at half-maximum (FWHM) of 2.6 mm. At a distance of 8 cm from the center, the PSF is elliptical with a transverse FWHM of 2.7 mm and a radial FWHM of 4.1 mm. These results demonstrate that the completed tomograph will provide a 300% improvement in spatial

resolution over our existing 280-crystal positron tomograph.

The need for an ultrahigh-resolution positron tomograph with multiple, close-packed rings has motivated the development of a new detector scheme where small BGO crystals are coupled in groups to phototubes for timing information and are coupled individually to silicon photodiodes for spatial and pulse-height information. We have demonstrated for the first time that silicon photodiodes can detect the scintillation light from BGO with an unprecedented combination of spatial and energy resolution. The detector concepts developed in this project will permit our group and other researchers to build improved positron tomographs for the benefit of medical research throughout the world.

(54) Transmethylation Kinetics in Schizophrenia
(k\$ 81)

T.W. Sargent

The goal of this project is to develop a brain-blood flow-imaging agent using positron-emitting 3.6-m ^{122}I from a ^{122}Xe - ^{122}I generator, for use in positron emission tomography (PET). The ^{122}Xe generator can be produced at a centralized cyclotron and shipped to other institutions, and the short half-life of ^{122}I will permit repeat studies at short intervals. The radiopharmaceutical will be a structural analog of 4-iodo-2,5-dimethoxyamphetamine (DOI), which we first demonstrated to undergo first-pass extraction into the brain. Nitrogen-substituted analogs of DOI may be produced by direct iodination of the N,N-disubstituted 2,5-dimethoxyamphetamine precursor in less than 1 minute. We will first identify the analog with the best characteristics by labeling with ^{131}I and studying its distribution. The reaction conditions for maximum speed, yield, and purity will then be determined, and a ^{122}Xe - ^{122}I generator system designed and built to produce the ^{122}I -labeled compound by automatic microprocessor control. Tests to validate brain-blood flow measurements against microspheres and iodoantipyrine will be followed by studies in patients with schizophrenia and other dementias using the Donner Laboratory 280-crystal PET system.

(55) Precision Scanning Microdensitometer Facility
(k\$ 166)

R.M. Glaeser

The equipment in this facility is being used primarily to digitize high-resolution electron micrographs and electron diffraction patterns, both of which are recorded on photographic emulsions. A major part of the electron crystallographic work is concerned with the structure and function of cell membrane proteins. Another electron crystallographic application is concerned with the structure analysis of thin crystalline plates of highly polymerized DNA. All of these projects are concerned with molecular structure analysis on basic problems that are currently of interest in the understanding of cell biology and biochemistry. In another type of application, the equipment will be used to digitize the position of heavy-ion "tracks" that are produced in thin plastic sheets and developed by solvent-etching. In this case the plastic films are used to record heavy-ion radiographs as part of an experimental program in tumor localization and heavy-ion radiotherapy.

(56) Experimental Medicine: Clinical
(k\$ 325)

T.F. Budinger

The objective of this program is to perfect noninvasive methods for measurement of biological functions of the brain, heart, and other human organs. The major medical science projects include: investigation of the physiological basis of brain disorders using emission tomography (PET and SPECT); development of techniques for the early detection of Alzheimer's disease and for studying the metabolic disorders associated with diseases such as schizophrenia; studies of low-density lipoprotein receptor distribution; and the evaluation of atherosclerosis.

Positron-emitting and single-photon-emitting radionuclides are used in conjunction with tomographic instrumentation, perfected at this laboratory, to quantitate specific metabolic functions such as blood brain barrier permeability, oxygen use, metabolism of sugars and amino acids, and receptor-site activity. A specific approach involves the acquisition of emission data on a moment-to-moment basis. With these data and a suitable physiological model we deduce parameters that reflect transport and metabolism of the specifically labeled radiopharmaceuticals. The methods include nuclear and organic chemistry, tomographic imaging procedures, autoradiography, stable-isotope detection methods, high-pressure liquid chromatography, and advanced computer kinetic modeling.

Major recent accomplishments include perfection of a noninvasive technique for measuring heart muscle blood flow; discovery of a specific pattern of glucose metabolism defect in patients with Alzheimer's disease; and development of a new very rapid computer technique for positron emission tomography kinetic data analysis.

New methodological results expected in the next three years include evaluation of the role of platelet accumulation in the neck and brain of individuals exhibiting prestroke symptoms; perfection of a method for quantitating low-density lipoprotein receptor activity in man using PET; delineation of the role of the blood brain barrier in Alzheimer's disease; and perfection of a method for evaluating brain blood flow using iodinated or fluorinated phenylalkylamine compounds.

Unique experimental approaches to atherosclerosis and aging are implemented by the application of high-technology emission imaging approaches perfected at this laboratory.

(57) Metabolism in Brain Disorders
(k\$ 149)

T.W. Sargent

This program is dedicated to use of advanced radioisotope methodology for investigation of human mental disorders. Schizophrenia and Alzheimer's dementia are tragic diseases that afflict a large percentage of our population and are enormous burdens in health care; discovery of basic causes could lead to more successful treatment or cure. The rationale is that schizophrenia is a genetically determined biochemical disorder whose basic cause may be discovered by *in-vivo* kinetic measurements of properly designed radio-labeled molecules. The Donner Positron Emission Tomograph (PET) is used for quantitative dynamic imaging of fluorine-18-fluoro-deoxyglucose (^{18}FDG) and ^{11}C -methionine. In well-diagnosed patients with schizophrenia, we have found significantly reduced uptake of FDG in the right frontal lobe of the brain, which, contrary to findings of other workers, is not changed by medication. We are now ready to begin a complex study of the kinetics of methyl-carbon metabolism in schizophrenia measured with [^{11}C -methyl]-methionine. In addition to dynamic PET studies of the brain, we will analyze expired $^{11}\text{CO}_2$ with our radiocarbon respirometer by which we first demonstrated abnormal methyl carbon oxidation in schizophrenia. We have successfully separated the major methyl carbon metabolites of methionine in a single HPLC system. This system will be used to identify and measure abnormal levels of the ^{11}C metabolites in the plasma of patients. We are developing a new iodo-amphetamine for brain blood flow studies based on the first iodo-amphetamine developed by us; it will be labeled with the 3.6-m positron emitter ^{122}I obtained from a 20-h ^{122}Xe generator. This will be the first brain blood flow agent available for PET studies, and we will use the 2.5-s-interval dynamic capability of the Donner PET to measure brain blood flow in Alzheimer's Dementia and schizophrenia. This will determine whether differences from normals that we have found in ^{18}FDG uptake in these diseases are due to metabolically less active areas of the brain or to decreased blood flow.

(58) Microdosimetry of Particulates
(k\$ 223)

T.L. Hayes

Research Objectives. This program investigates basic structural and chemical properties of the lung tissue and individual lung cells.

Rationale. The lung is a heterogeneous population of individual cells in a highly organized hierarchical matrix. Events, such as mutation and carcinogenesis, at the level of single cells, are basic to a better understanding of tissue, organ, and other whole organism responses.

Experimental Approach. Organizations of cells into neighborhoods, airways, and respiratory units in the lung are analyzed such that structural and chemical information is indexed by position along the airway. Precise correlation of structural information and elemental composition of individual cells is carried out through the application of frozen-hydrated-specimen techniques and x-ray microanalysis.

Progress. Surfaces of individual alveolar septa analyzed with the Scanning Electron Microscope (SEM) can be correlated with Transmission Electron Microscope (TEM) analyses of the interior of the identical septum. Alveolar walls preselected from SEM maps and then excised have been transilluminated with the High Voltage Electron Microscope (HVEM). A study of the patency of the pores of Kohn in the frozen-hydrated state shows that all pores are closed and not available for collateral ventilation.

Significance. The patency of the holes in the alveolar wall, important to collateral ventilation, is significant in interactions of foreign particles and gases with the lung and in chronic respiratory diseases. The question of the continuity of the alveolar surfactant layer should be aided by this work. Low-temperature analytic methods yield basic structural and chemical information important to a better understanding of the interaction between lung cells and their extracellular matrix.

Future Directions. Continuing efforts will be made to answer basic questions of lung-cell structures and microchemistry. Emphasis will be placed on the studies of variance in individual lung-cell ionic composition and analysis of the structure of the alveolar wall.

(59) Biological Structure Analysis by Electron Microscopy
(k\$ 453)

R.M. Glaeser

We will continue to use the technique of electron diffraction and high-resolution electron microscopy, complemented by biochemical and biophysical studies, to determine molecular structures of several membrane proteins. We will devote a significant effort to finding a technical solution for the specimen flatness problem to obtain high-resolution images at large tilt angles for three-dimensional reconstructions. Parallel to this effort, we will also use the Fourier difference technique to localize heavy atoms inserted at sites produced by enzymatic cleavage and at the tyrosine reactive sites in the in-plane projections. Information gained will be used to reduce the number of models currently possible. A working model can be proposed and tested for agreement between the calculated diffraction intensities and the ones actually observed.

We will attempt to crystallize aspartate chemoreceptor protein and its aspartate-binding N-terminus fragment. We will also reinitiate our study of the F_0 complex of the ATPase. Our earlier crystallization was limited to the smallest subunit (c) of F_0 . We now believe that more information can be gained by studying the entire F_0 complex, since recent studies suggest that all 3 components of F_0 are essential for its proton-translocating activity.

(60) Resonance Studies in Photosynthesis
(k\$ 64)

A.J. Bearden

The processes by which green plants and photosynthetic bacteria convert absorbed light into chemical free energy efficiently continue to require investigation by modern spectroscopic techniques. The elucidation of the many steps by which photon absorption, the production of increasingly stable charge separation (oxidized electron donors and reduced electron acceptors), and finally the use of the energy of charge separation to drive ATP synthesis and the production of reducing equivalents requires the application of a wide variety of experimental methods along with careful control of the biological media. Our use of short laser-derived light flashes and time dependent electron paramagnetic resonance (EPR) spectroscopy has permitted significant advances to be made in understanding the early photophysical and photochemical processes in green-plant photosynthesis. Although EPR spectroscopy cannot compete with information gained on a picosecond time scale by optical absorption measurements, important information about EPR-detectable species such as the reaction-center chlorophyll (P700) and a seemingly overcomplex array of a series of electron acceptors can be gained on the microsecond-to-nanosecond time scale by judicious use of the inherently slower EPR method. Dual-laser flash excitation and the subsequent measurement of acceptor type and concentration has afforded a model of charge recombination for Photosystem I in chloroplasts. Our approaches are based heavily on the use of pulsed and saturation-recovery EPR, partially oriented samples, and the positioning of chemically inert paramagnetic "relaxers" at specified positions in oriented biomembranes. The effects of these added paramagnetic entities on the relaxation times and other properties of EPR signals from known participants in photosynthetic charge transfer and electron-transport chain components gives valuable information about position and orientation. Specifically, our investigations are aimed at providing answers to the question of the order of physiologically active acceptors in green-plant (chloroplast) Photosystem I, the importance of tunneling as a participant in electron-transport processes, and continued measurements of orientation and position of membrane-bound electron-transport components in chloroplasts. Associated problems for theoretical study included extension of the Jortner-Hopfield theory of tunneling to cover more detailed experimental work on biological tunneling, investigation of the theoretical basis for protein conformation substates at low temperature and their role in biological energy flow, and continued new methods of EPR spectroscopy in application to photosynthesis.

(61) Hemopoietic Cellular Proliferation and Its Regulation, Training Grant
(k\$ 88)

S.N. Ebbe

The purpose of the program is to train individuals in research aspects of hematopoiesis. The trainees will be physicians, scientists with a Ph.D. in biological or physical science, or predoctoral students in medical physics, physiology, or the like.

The emphasis in this program will be on the one-to-one association of trainees with preceptors who are established investigators and have an interest in developing the technical skills and critical judgment of young potential investigators. The assigned or chosen research work will be as independent as appropriate for each individual trainee. Seminars, in which both trainees and staff will participate, and individual library research will occur concurrently. Post-doctoral trainees will be encouraged to enroll in a small number of formal lecture and laboratory courses. Predoctoral trainees will enroll in the courses required by their major.

The expertise of the staff provides a broad knowledge of hematopoiesis, so trainees may select areas of interest to them: kinetics and physiology of pluripotent stem cells, granulocytopenia, lymphocytopenia, erythropoiesis, megakaryocytopenia, cellular immunology, regulation of cell proliferation, transplantation biology, cell culture, cell deformability, and

application of nuclear-medicine and electronic techniques to cell biology.

(62) Cardiovascular Flow and Metabolism, Training Grant
(k\$ 71)

T.F. Budinger

This is a program for training physicians, physicists, chemists, and biologists in pre- and postdoctoral categories in the techniques appropriate for cardiovascular research using advanced instrumentation techniques, radiopharmaceuticals, and analytical methods.

Physicians and physiologists will gain a foundation in applied physics, and mathematicians and physicists will acquire sufficient background in physiology and medicine to enable them to engage in independent or team research involving methods of diagnosis and investigation used in cardiovascular research. Upon completion of this program, trainees will be able to initiate independent research inquiries or join research teams where their newly acquired skills are of vital need, e.g., nuclear magnetic resonance imaging, microsphere circulation studies, autoradiography, and electron microscopy. Physicians will have acquired sufficient academic exposure and research indoctrination to qualify for academic or research staff positions in medical schools.

The methods of training include a tutorial scheme in which concentration during the initial six months is distributed in the following areas: basic medical physics and applied chemistry; gamma counting and spectroscopy; nuclear-medicine instrumentation for imaging; NMR imaging instrumentation; positron emission tomography; ultra-sound imaging; radioimmunoassay; radiopharmaceutical preparation using short-half-life isotopes; autoradiography; microsphere circulation techniques; computer methods for kinetic analysis and three-dimensional reconstruction; animal surgery; and clinical cardiology, lipidology, and hematology. After this initial six months, independent projects are assigned and formal classwork is arranged according to the needs of the individual. The research project will be part of a team effort so that the trainee will have continuous interaction with other trainees and more than one preceptor.

(63) Lipoprotein Methodology, Structure and Function, Training Grant
(k\$ 90)

T.M. Forte

The purpose of this program is to train postdoctoral fellows and graduate students in the investigation of lipoprotein structure and function. Our major expectation is that the trainees will be able to pursue independent careers in arteriosclerosis research or related fields.

Postdoctoral trainees participating in this program are required to have backgrounds emphasizing biochemistry, physiology, or biophysics. Training will be carried out within the research framework of the Lipoprotein Group in the Donner Laboratory. This group consists of four participating established investigators and represents expertise in the following basic areas of lipoprotein research: development of methodology for identification and quantification of lipoprotein subpopulations; characterization of the physical-chemical properties of lipoprotein subpopulations; delineation of the metabolic interconversions and interrelationships among lipoprotein subpopulations; and application of the physical-chemical and metabolic information to the basic problem of atherogenesis at the cellular and intact animal level. Trainees will be introduced to each of these areas of research during a period of orientation and subsequently will proceed to an in-depth research program in one of them. Informal weekly meetings of staff and trainees will be held for discussion of current problems in lipoprotein research. Formal seminars (Lipoprotein Research Seminars) are held biweekly. At these seminars staff and trainees describe their work in progress or discuss recent publications relevant to their work. Trainees are also encouraged to take advantage of the many resources, such as special seminars and courses, available on the Berkeley Campus of the University of California.

(64) Jackson State University Collaborative Research
(k\$ 38)

D. Chan

This research project is being conducted as one of the aspects of the collaborative research agreement between Jackson State University and LBL. The objective of the study is to investigate the synthesis and turnover of components associated with the extracellular matrix of cultured normal and virally transformed tendon fibroblasts. The study is an extension of work carried out by Dr. Chan while she was a visiting scientist at LBL in FY 1982 and FY 1983 under the same collaborative agreement.

CENTER FOR ADVANCED MATERIALS

A.G. Evans, Associate Director (Acting)

The Center for Advanced Materials (CAM) was established October 1, 1983 at the Lawrence Berkeley Laboratory to help meet the need for major research efforts in areas of materials science that are vital to U.S. industrial strength. High technologies depend critically on the development of sophisticated new materials and the ingenious exploitation of their physical, chemical, and biological properties. In many areas, however, progress is blocked by our insufficient understanding of the underlying basic materials science.

At CAM, strong interdisciplinary teams of investigators undertake applications-oriented basic research aimed at solving these problems with the view of transferring essential new technologies to the industrial sector, typically within 5 to 15 years. Thus, a close working relationship with industry is a major aspect of the CAM program. It is maintained through the naming of industrial scientists to a Scientific Policy Board, which provides overall direction to CAM, and to program advisory boards, which comment on research progress and the plans of the individual programs. In addition, CAM has established programs to allow scientists from industrial research laboratories to work in CAM laboratories for extended periods. Another component of the CAM effort is the training of large numbers of graduate students and postdoctoral fellows for materials science research positions both in industry and academia. The coupling of the resources and capabilities of a national laboratory with the expertise of academic and industrial research scientists, in conjunction with the training of new generations of materials scientists and postdoctoral fellows, sets a model for productive collaboration within the research community.

The total funding for CAM in FY 1984 was k\$ 2800. The program areas are described below.

(1) Electronic Materials Program

E.E. Haller

The purpose of this program is:

1. To gain a basic understanding and control of the parameters that affect the quality of large-diameter III-V compound semiconductor single crystals, epitaxial films, and interfaces.
2. To develop and implement novel and advanced characterization techniques.
3. To further the understanding of the large variety of defects and defect interactions on an atomic scale.

A theoretical and experimental program has been started in three major areas: bulk crystal growth, thin films and interfaces, and characterization. In bulk crystal growth, the theoretical effort has concentrated on heat-flow and mass-flow modeling for Czochralski and Bridgman furnaces.

The characterization effort has produced the first GaAs lattice images using the atomic resolution microscopes at LBL's National Center for Electron Microscopy. These images verify the predicted asymmetry in the electron density around the As and the Ga atoms. Synchrotron

radiation at the Stanford Synchrotron Radiation Laboratory and at Cornell University has been used to image dislocations, stacking faults, and precipitates in wafers of GaAs. Unknown clusters have been discovered in indium-doped GaAs single crystals. In addition, a dedicated Electron Paramagnetic Resonance Spectroscopy facility has been established and has been used to record antisite spectra in neutron-irradiated and pure, semi-insulating material.

(2) Advanced Instrumentation for Surface Science

J. Clarke

This program is intended to develop new techniques and instruments for the study of surfaces.

A scanning tunneling microscope has been constructed. Samples can be introduced into and withdrawn from the ultrahigh vacuum chamber without breaking vacuum, and the microscope operation and data collection are under computer control. Present resolution is about 10 Å, and it is expected that atomic resolution will soon be achieved. Problems that can be investigated with this type of instrument include surface reconstruction, the location of adsorbed atoms and molecules, the structure of as-grown semiconductors, and the effects of laser annealing.

Linear and nonlinear optical studies of polymers on organic and metal surfaces and surfactants on metal and metal-oxide surfaces using a variety of techniques such as surface plasmons, total reflection, second- and third-harmonic generation, and Raman spectroscopy are also being performed. The first observation of the angle of orientation of molecules of an adsorbed monolayer, specifically surfactant molecules at a water-air interface, has been achieved using the second-harmonic-generation technique.

A system for the study of far-infrared absorption by atomic and molecular adsorbates has been assembled and tested. The substrates on which the adsorbates are deposited are attached to doped Ge thermometers and mounted in a vacuum can at liquid-helium temperatures. The absorptivity of the surface is determined by scanning the frequency of the incident radiation and measuring the resulting rise in surface temperature.

(3) Polymers and Polymer Composites Program

M.M. Denn

The goal of this program is to develop a sound scientific basis for the prediction and control of microstructure in the processing of high-performance polymeric materials. Microstructure control is essential to produce shaped objects with sufficient strength, thermal stability, and chemical resistance to allow their use as lightweight structural elements in a variety of environments.

The program is focusing on three classes of polymeric materials having considerable applications potential: liquid-crystal polymers, block copolymers, and short-fiber polymer composites. We are also interested in three processing areas that are relevant both to the particular materials types selected for study and to broader subject areas within the field: coprocessing, structure control through polymer-solvent-nonsolvent interaction, and molecular-weight distribution control through polymerization reaction engineering.

Experimental techniques include solid-state nuclear magnetic resonance spectroscopy, x-ray diffraction, rheological characterization, a new laser-speckle method, and microscopy.

Theoretical approaches include classical lubrication theory, colloidal nucleation theory, and Flory Huggins theory and the development of new finite-element methods for the analysis of flows of rheologically complex materials.

(4) Advanced Structural Ceramics

L.C. De Jonghe

The Ceramics Program is a long-range interdisciplinary research effort that has the objective of broadening the scientific base needed for the development of high-temperature structural ceramics. The central scientific issues are: how do microstructural heterogeneities arise and affect mechanical properties of ceramics and how can these be manipulated to fully exploit the potential of ceramics in high-temperature structural applications. The work is focused on fundamental theories and generic phenomena. It thus complements programs elsewhere that are focused on the development of specific high-temperature structural ceramics.

At present, four interrelated activities are addressed: (1) the experimental and theoretical study of static and dynamic colloid behavior in relation to slip casting and injection molding; (2) the study of the development of microstructural heterogeneities arising at the particle level, as related to continuum treatment of sintering stresses and their consequences; (3) the establishment and verification of high-temperature creep-failure theories; and (4) the study of fundamental aspects of erosion and wear.

Present studies include the development of multiparticle interactions in concentrated colloids, incorporating surface chemistry; transmission electron microscopy characterization of silicon carbide and nitride powders; chemical modification of silicon nitride powder surfaces and surface characterization by secondary ion-mass spectrometry and photoelectron spectroscopy; two-dimensional studies of multiparticle densification at the particle level; examination of creep sintering by means of a newly developed loading dilatometer; the study of newly discovered creep rupture by shear band cavitation at high temperatures; and the relation of these phenomena to microstructural and microchemical heterogeneities.

(5) Catalysis Program

G.A. Somorjai

The major emphasis of this program is the synthesis, characterization, and evaluation of new catalysts based on synthetic zeolites and other microporous crystals, transition-metal compounds, and transition-metal complex catalysis in novel matrices. This research offers considerable promise of finding new, lower-cost catalysts with increased selectivity and resistance to degradation during use in industrial conditions. Additional attention is being placed on catalytic reactions stimulated by plasma or laser excitation.

Zeolites. Zeolite catalysts are being synthesized and characterized using techniques such as high-resolution electron microscopy, extended x-ray fine structure, solid-state nuclear magnetic resonance, and adsorption studies. Particular attention is being given to understanding the relationship between synthesis conditions and zeolite structure with emphasis on the nucleation state. The coordination of silica and alumina and the effect of templates are being investigated.

Transition-Metal Compounds. The initial focus here is being placed on the carbides and nitrides of the Group IV through VI transition metals and some Group VII silicides. Both supported and bulk configurations are under investigation. Structures are being determined as are catalytic properties.

Novel Materials and Reaction Conditions. Organometallic molecules anchored to organic and inorganic polymer surfaces are being synthesized, and their potentially unique catalytic properties will be evaluated, e.g., as films placed on electrodes.

CHEMICAL BIODYNAMICS DIVISION

G.C. Pimentel, Associate Director

(1) Hydrocarbons and Energy from Plants
(k\$ 150)M. Calvin
J. Ottvos

This project involves the study of green plants as renewable resources for hydrocarbon production, with the major emphasis on the investigation of terpenoid-producing species. Terpenoids are a major class of natural products that are found in many plants. They are often in a highly reduced state, either as pure hydrocarbons or with a sufficiently low degree of oxygenation so that they can be catalytically reformed to pure hydrocarbons. This very large and diverse class of plant metabolites, therefore, represents a potential source of chemical feedstock material and/or high-energy liquid fuels.

Plants that produce hydrocarbon-like materials such as terpenoids are quite diverse in their chemical composition and possibly in their mode of biosynthesis of terpenes. Useful products can be stored and synthesized in various plant parts. *Euphorbias* and *Asclepias* store reduced terpenes in their latex, whereas some trees can be tapped for light resins or oils of various chemical composition. To aid in the selection of species for study and also in the development of appropriate processing procedures, more knowledge of plant chemistry is required.

The level of biological organization to be emphasized in this program is the single plant and its constituent organs and tissues. The philosophy of the program is to obtain information concerning critical issues at the plant level so that agronomic trials in subsequent years can be undertaken with a sound foundation. Such agronomic field trials, however, are outside the scope of this project as are genetic engineering methods aimed at enhancement of terpenoid production.

(2) (a) Biophysical Chemistry

(a) M.P. Klein

(b) Genetic Elements Controlling the Growth of Cells in Culture
(k\$ 240)

(b) J.C. Bartholomew

(a) The objectives of this research are to achieve a basic understanding of the molecular consequences and correlates of cellular transformation and to develop methods for determining the pertinent molecular and cellular parameters associated with these processes. Measurements of cellular metabolism, bioenergetics, and cellular membrane dynamics and interactions between membrane and extracellular surfaces are performed *in vivo* by a variety of biophysical spectroscopic methods. Such measurements are anticipated to reveal the origins of the quantitative differences observed between normal and transformed cellular metabolism. These measurements will have a significant implication for both whole-body nuclear-magnetic-resonance imaging and for combined imaging and spectroscopy. It is planned to determine how membrane mobility is modified by tumor-promoter-induced protein reorganization. The detailed metal environments of the Fe and Mn forms of superoxide dismutase will be studied by single-crystal electron paramagnetic resonance and electron-spin echo spectroscopy.

(b) It has been well documented that cells growing in culture maintain various forms of growth control. In general, transformed or malignant cells have relaxed growth control properties when compared to nontransformed or nonmalignant cells. The primary growth control point in the cell cycle is active in G₁ just after the cells have divided. This regulatory point is responsive to factors added to the medium that promote the maintenance of cells in the replicative cycle. In some cases these factors have been identified such as platelet-derived growth

factor, epidermal growth factor, fibroblast growth factor, etc., and at least in one case, the growth factor gene has been shown to be related to known *onc* sequences resulting in the increased growth characteristic of malignant transformation. These studies suggest that *onc* sequences may normally be involved with the regulation of cell growth. Our preliminary experiments have shown that c-myc will stimulate DNA synthesis in CV-1 cells approximately four-fold.

(3) Mutagenesis-Fundamental Chemistry
(k\$ 130)

J.E. Hearst

The objective of this research is the determination of molecular mechanisms of mutagenesis. The approach will be to use site-specific modification of an infectious M13 viral DNA molecule by reaction with a polynuclear oxygen-containing molecule, a psoralen, or a polynuclear aromatic heterocyclic amine.

In the past year the techniques of dideoxynucleotide DNA-sequencing procedures have been perfected. Several site-specifically modified M13 molecules have been formed, all of which have a psoralen added to a thymidine at one site in the genome. Furthermore, the stereochemistry of the adduct at each of those sites is known. The site of modification has been selected to be in the middle of a single hit restriction site in the intergenic region of M13, so no mutations that are lethal to the virus are expected. Transfection experiments are being performed at present.

In future studies replicative-form DNA that is isolated from the transfection will be restricted with the appropriate enzyme, and site-specific mutants will be identified as resistant to restriction. A second round of transfection will allow for the cloning of these mutant viral genomes. They will be sequenced in the mutated region, and the resulting sequence changes will be cataloged.

(4) Cellular Aspects of Chemical Carcinogenesis
(k\$ 230)

J.C. Bartholomew

Over the last few years our studies have concentrated on the inhibitory effects of benzo[a]pyrene diol epoxide on DNA synthesis in mammalian cells. These studies were generally carried out at high doses of this chemical to do biochemical and cell-kinetic analyses. Our new studies use low doses of chemicals and have the goal of determining the effect of modifications in DNA on genome stability. We are studying the replication, recombination, and rearrangement of specific DNA sequences that are either present in the genome of the cells or as exogenously added DNA vectors. With exogenously added DNA, the DNA is modified *in vitro* with benzo[a]pyrene diol epoxide and transfected into mammalian cells. We are following the fate of these molecules in normal human fibroblasts, as well as in repair-deficient XP cells, to determine if repair functions are important in the replication and recombination of carcinogen-treated DNA's. All of these studies are closely tied to other work at Chemical Biodynamics designed to investigate the effect of chemical modification of DNA on structure.

(5) Structural Biophysics
(k\$ 140)

S.-H. Kim

The overall objective is to understand, at the molecular level, the interaction of DNA and proteins with toxic materials in the environment. Methods include x-ray crystallography, nuclear magnetic resonance (NMR), and biochemical and molecular biological techniques. Three systems are used for this purpose:

1. Psoralens are natural compounds that interact with DNA and damage DNA on UV irradiation. We plan to study the structural aspects of DNA damage by x-ray

diffraction and NMR techniques combined with DNA synthesis.

2. Netropsin and Distamycin are a class of antibacterial, antiviral, and antitumor drugs that bind to DNA without covalent binding or intercalation. Our goal is to study DNA-structure distortion induced by these drugs, a factor that may be important in understanding their drug activities.
3. When mammals are exposed to heavy toxic metal ions, a class of proteins called metallothioneins is produced, and they bind to the metal ions and remove them from the bloodstream. Our objectives are (a) to have a basic understanding of how metallothioneins bind a variety of metal ions with different coordination geometry and (b) to make altered metallothioneins for certain metal ions that are especially harmful to human beings.

(6) Photoconversion/Artificial Photosynthesis
(k\$ 920)

G.C. Pimentel
M. Calvin
J. Otvos
J. H. Clark

This program encompasses research directed at a fundamental understanding of electronically excited molecules with special attention to features that relate to the storage of photon energy in the form of high-free-energy chemical bonds. The first subtask, under the direction of M. Calvin and J. Otvos, investigates synthetic systems that convert solar quanta into stored chemical energy, focusing on effective photo catalysts and photoelectron transfer across phase boundaries in aqueous media. Present thrusts are toward increased quantum yields, increased free-energy storage, elimination of sacrificial electron donors in favor of oxidation catalysts that will either produce O_2 or convert an organic substrate to an energy-rich product. In a new direction, the electrochemical and photochemical reduction of carbon dioxide is being explored. The second subtask, under the direction of G.C. Pimentel and H. Frei, generalizes artificial photosynthesis to other solvent media and energy-storage reactions other than oxidation-reduction. Emphasis is placed on clarifying the distinctive chemistry of electronically excited atoms and molecules, electronic energy transfer, and energy relaxation processes in nonaqueous, condensed, and cryogenic environments. Using laser spectroscopic techniques, electronic hypersurface mapping is being explored. The third subtask, under the direction of J. Clark, exploits picosecond visible/UV absorption, fluorescence, and resonance Raman spectroscopic techniques to determine the kinetic behavior in real time of excited-state proton transfer and electron transfer reactions. These techniques are now being applied to excited-state proton transfer in substituted naphthols, intramolecular charge transfer dynamics in tris (bipyridine) ruthenium II, and energy transfer rates in photosynthetic cyanobacteria.

(7) Energy Conversion in Photosynthesis
(k\$ 287)

K. Sauer
M. P. Klein

Our objective is to elucidate basic principles that underlie the conversion of solar energy into chemical energy as it occurs in photosynthetic organisms. We are using spectroscopic approaches to explore the nature of the photosynthetic light reactions, the composition and organization of photosynthetically active membranes, and the mechanism of water oxidation to molecular oxygen in higher plants.

The following are recent significant accomplishments.

1. Fluorescence decay kinetics measurements using single-photon timing indicate that
 - a) the state of chemical reduction profoundly influences the amplitude of the slow decay components of fluorescence from chloroplasts, but not the fast or middle

components.

- b) heterogeneity of Photosystem 2 reaction centers is evident.
 - c) changes in decay kinetics accompany the development of chloroplast membranes.
 - d) thylakoid membrane protein phosphorylation influences the decay pattern, reflecting changes in excitation migration.
2. Electron paramagnetic resonance (EPR) of unpaired electrons, radical pair, and triplet species in chloroplasts indicate that
- a) the orientation and temperature dependence of EPR transients characterize two primary acceptor species in Photosystem 1.
 - b) kinetics of the rise of the rapid light-induced Signal II and the decay of P680+ show that the two components are immediately adjacent to one another in Photosystem 2.

(8) (a) Mapping Photosynthetic Genes
(b) Light Regulation of Photosynthesis
 (k\$ 194)

(a) J.E. Hearst
 (b) J.C. Bartholomew

(a) The objective of this subtask is the determination of the primary molecular events in the fixation of electromagnetic radiation by photosynthetic bacteria and by plants. Utilizing transposon mutagenesis, we have identified and phenotypically characterized more than forty mutations in the photosynthetic genes of *Rhodospseudomonas capsulata*, a photosynthetic bacterium. Our approach is to learn all we can about the biochemistry of photosynthesis by a careful characterization of these mutants. We have also identified and sequenced the genes of the H, L, and M subunits of the reaction centers of *R. capsulata*. We have sequenced an additional 5000 nucleotides of DNA with apparent control function, and we are searching for the protein products that are coded by these sequences.

We intend to establish functions for the control genes mentioned above. We also intend to identify the biochemical blockages in carotenoid and bacteriochlorophyll biosynthesis in the many mutants that have been isolated. The sites of quinone binding in reaction centers are to be identified using the techniques of site-specific mutagenesis.

(b) Even though the chloroplasts of photosynthetic organisms contain their own genome, many of the functions carried out in the organelle are encoded in the nucleus. Some of the proteins that function in chloroplast are encoded partially in the chloroplast and partially in the nucleus. The expression of both these genomes is regulated by light. Light stimulates mRNA synthesis and DNA synthesis in *Euglena gracilis*. Presumably, this light response is mediated by photopigments in the cells that receive the light and convert it into a signal that controls nucleic acid activity in both the genome compartments. We have a series of bleached mutants of *Euglena* that lack various photopigments as well as have different levels of chloroplast DNA. We are using these mutants to study the involvement of the photopigments and chloroplast DNA in the stimulation of nuclear DNA and ribonucleic acid (RNA) synthesis. These studies are designed to help us understand the factors involved in the coordinate regulation of the genes in the two physically distinct compartments.

(9) Plant Biochemistry
(k\$ 349)

(a) J. A. Bassham
(b) H. Rapoport

(a) Mechanisms of regulation of expression of photosynthetic and biosynthesis carbon paths in green plants are elucidated. Investigations are made of both the control of gene expression and of regulation of enzyme activities in response to physiological conditions. Gene expression in various tissues and as a function of development is evaluated through measurements of mRNA, polypeptides (using protein blot methods), and enzyme activity. Restriction fragments from nuclear DNA are probed with DNA identified with key enzymes as a first step toward locating these genes in the plant genome and also determining nuclear mechanisms of regulation of gene expression. Other studies are conducted using plant cell tissue culture, isolated protoplasts and organelles, and techniques of flow cytometry, somatic fusion, and plant regeneration as tools for examining gene transfer.

(b) A complete understanding of the chemistry of phytochrome is sought to facilitate full understanding of the role of light in regulation of gene expression in green plants. The chemical structure of phytochrome is being determined, including the nature of attachments of chromophore to protein, by stereospecific synthesis of model chromophores. Knowledge of such mechanisms is required for future improvement in plant growth and quality based on genetic engineering at the molecular level.

(10) National Tritium-Labeling Facility
(k\$ 435)

R. M. Lemmon
H. Rapoport

This facility is available to scientists throughout the country who wish to prepare tritiated compounds at very high specific activities and radiopurities that are not available commercially. Research at the facility involves the study of novel methods of introducing tritium into organic compounds. Such methods include generation of active tritium radicals and ions in a microwave plasma that is directed toward selected targets. Mechanisms such as addition, substitution, and dehalogenation by the excited tritons are under study. The facility also functions as a training laboratory for handling large quantities (i.e., hundreds of curies) of tritium safely and for learning the latest techniques for purifying and storing radioactively labeled compounds.

COMPUTING DIVISION

L.T. Kerth, Associate Director

(1) Advanced Computer Concepts
(k\$ 315)

J. Sventek

This program concentrates on research problems concerning the effective use of distributed computer systems. A major thrust of the distributed systems research program is the performance measurement of local-area network interconnection hardware, performance measurement of communication protocol implementations utilizing this hardware, and subsequent analysis of the measurements using simulation and other modeling techniques. As a result of this work, realistic estimates of local-area network performance in DOE environments can be made; additionally, the enhancements to network hardware and software necessary to achieve required performance characteristics can be determined.

In line with the current DOE emphasis on high-speed computing, some effort is being redirected to the application of the above modeling techniques to performance aspects of parallel computer architectures. Performance-model results for variables such as cache size, memory bandwidth, and interconnection networks will provide essential input for DOE-sponsored parallel architecture development projects.

Another facet of the current program involves research into scientific work station computers, which provide a hospitable environment for scientists to develop and test production programs prior to their execution in high-speed computing environments. Particular emphasis will be placed on remote execution and debugging of FORTRAN programs, along with incorporation of state-of-the-art program development environments (such as the DOE-sponsored TOOLPACK). The ultimate goal of such work is to permit scientists to use all of the computational tools at their disposal from within an environment tailored to their needs. Such an approach also relieves the developers of high-speed computing systems from the development of interactive user-interface software, permitting more resources to be devoted to the enhancement of the systems as computation engines.

(2) Information Analysis Techniques
(k\$ 525)

A. Shoshani

Research in this program seeks innovative approaches to the management, manipulation, and display of large, "statistical and scientific data bases." Statistical data bases are primarily collected for the purpose of providing statistical summaries, such as energy consumption and production. Scientific data bases result from experiments and simulations of physical phenomena, such as the collision of particle beams or heat transfer in buildings. These data bases have requirements that cannot be easily supported by existing commercial data-management systems. The purpose of the data-management research program is to develop techniques that are tailored to the special characteristics and usage of such data bases.

In the past several years, the research emphasis was on statistical data bases. During the next year scientific data bases will be investigated with the goal of determining which statistical data-base techniques can be applied to them as well. In addition, several requirements that are specific to scientific data bases will be identified. Preliminary studies indicate that the following areas of research could provide significant results. The "physical organization" area is concerned with compressing data and accessing them efficiently, as well as organizing and managing files on secondary storage. The "modeling" area provides a convenient way to view complex data sets and access them efficiently. This is particularly important for scientific data

bases where the data associated with the setting of an experiment and the log of instruments behavior need to be associated with the measured data.

Another aspect of the research program is to investigate how to use parallel processors efficiently for statistical and scientific data bases. The promising research areas are in minimizing the synchronization cost between the processors that access the same data base and in determining the best partitioning of a data base over multiple disks for efficient parallel processing.

(3) Populations at Risk to Environmental Pollution (PAREP)
(k\$ 175)

D.W. Merrill
S. Selvin

The PAREP project focuses on the collection, analysis, and interpretation of data pertaining to relationships between human health and environmental pollution. The PAREP project data base forms an integral part of the Socio-Economic Environmental Demographic Information System (SEEDIS), which also provides access to large quantities of socio-economic data, population counts, environmental data, and other relevant information. SEEDIS allows the user to extract, analyze, and display selected data for use in specific epidemiologic investigations.

In FY 1985-86, the PAREP project will continue to collect health, environmental, and socio-economic data; to develop analytic techniques; and to consider important epidemiologic issues. Specifically, the following areas will be addressed:

1. Epidemiologic investigation of mortality.
2. Epidemiologic investigation of cancer incidence.
3. Equal-density geographic transformations (cartograms).
4. Epidemiologic consequences of employing census data.
5. Intercensal population estimates.
6. U.S. mortality, 1950-1978.

(4) Scientific Information Management
(k\$ 150)

J. McCarthy

This project is a research and development effort to make a broad range of scientific data more easily accessible to DOE users. The project is currently designing and developing an experimental prototype, distributed-computer system to store, index, search for, and retrieve diverse types of scientific data, including numeric tables, formulae, symbols, graphic images, and bibliographic citations from a variety of data bases. The goal is to provide users at DOE and DOE-contractor facilities with appropriate computer tools to find and access such data in the same way that they currently can find and access bibliographic citations using systems such as RECON and DIALOG.

The initial prototype system will focus primarily on materials-properties data of interest to a selected group of design engineers and analysts at DOE laboratories. It will be accessible via the ARPANET and local area computer networks within individual laboratories. A computer data base of materials-properties data offers several potential advantages over current methods of distributing such information via regular printed materials: it shortens the publication cycle and makes recent findings more quickly available; it facilitates searching for information in a wide variety of ways, which are not limited to terms that happen to have been indexed; it facilitates direct transmission of numeric and nonnumeric information that can be used directly by other computer programs for design and analysis; and it minimizes error-prone manual methods for entering and checking data.

LBL is cooperating in this project with a number of individuals from other organizations across the country, including DOE's Office of Scientific and Technical Information (which is

also the project sponsor), National Bureau of Standards' Office of Standard Reference Data, General Electric Corporate Research Division, Sandia Corporation, and Battelle Columbus Laboratory.

**(5) Socio-Economic Environmental Demographic
Information System (SEEDIS)**
(k\$ 1500)

C. Quong
H. Holmes

Research and development in the areas of distributed information systems technology, data management, and information display and analysis are collaboratively supported by DOE's Office of Energy Research and the Department of Labor Employment and Training Administration. SEEDIS consists of a very large integrated data base and sophisticated analytical and information-display capabilities. The objective of the SEEDIS program is to establish a coherent and comprehensive computer-based information system for application to epidemiological studies, environmental impact studies, and other socio-economic analyses. An experimental, homogeneous network of minicomputers, the Distributed Computer Network (DCN) has been developed to provide a basis for extension of SEEDIS into the area of distributed information technology.

EARTH SCIENCES DIVISION**T.V. McEvilly, Associate Director****(1) Geosciences Program**
(k\$ 1500)

T.V. McEvilly

This is a broad program in fundamental research to further the scientific basis and improve the technology for recovery and use of fossil fuel and strategic minerals from the earth, extraction of energy from hot brines and magmas, and safe disposal of radioactive wastes. Program topics at LBL include the dynamics of subsurface reservoirs, the physical behavior of fractured, fluid-saturated rocks under high temperatures and pressures, the physical and chemical properties of magmas, the thermodynamics of electrolytes, the generation and migration of petroleum compounds, the occurrence of abiogenic methane, the reactions between rock-forming minerals and groundwater, improved combustion processes, and state-of-the-art geophysical investigations employing unique electromagnetic and seismic methods. The seismology research, which includes the Center for Computational Seismology that provides modern computation facilities and seismological software to advance the art of seismic interpretation, offers improved computational methods to researchers and exposes students to state-of-the-art analytical techniques. Other studies pursue the more long-range goals of the Geoscience Program: to better understand the structure and dynamic processes of the earth's deep crust and how they may influence energy programs. In this respect, investigations associated with the Continental Scientific Drilling Program (CSDP) are under way, including geochemical and geophysical studies in the Long Valley Caldera of eastern California, similar work in the Valles Caldera of New Mexico and the Salton Trough of southern California, and the compilation of comprehensive data bases on topics of interest to the CSDP scientific community.

(2) Geothermal Research
(k\$ 900)

M.J. Lippmann

This is an integrated field, laboratory and theoretical program to develop techniques to delineate and characterize low- to high-temperature hydrothermal-geothermal systems to advance the state of the art of geothermal reservoir definition. A geophysical segment of this program involves the development and testing of instrumentation, field techniques, and data processing and interpretation. Under investigation are advanced electromagnetic techniques, improved passive-seismic technologies, and the application of modern seismic-reflection data acquisition and processing to geothermal reservoir delineation and mapping. A second focus of the program is to develop well-testing techniques, laboratory methods, and mathematical modeling tools to analyze and evaluate geothermal reservoirs. Under study are various reservoir engineering methods to characterize and simulate the dynamic behavior of liquid- and vapor-dominated systems under natural and exploitation conditions, assuming either constant or changing fluid compositions or fracture or porous reservoir rock conditions. Laboratory work includes the measurements of relative permeabilities of rocks under high-temperature conditions and the study of fluid flow through fracture networks. A further extension of the geothermal research program is to improve our capability to numerically simulate the response of geothermal systems to cold wastewater injection. These methods, developed to monitor and predict the behavior of the reservoir, will allow optimizing the design of fluid-injection operations for extracting the heat stored in the subsurface. The techniques and instrumentation developed under this program have been successfully field-tested at different geothermal sites, and the modeling results have matched favorably against data from U.S. and foreign geothermal fields.

(3) Development of Hydrofracture Technologies
(k\$ 700)

H.F. Morrison
T.V. McEvilly

Hydrofracturing is a common technique used in the oil and gas industry and, to a much lesser degree, in geothermal and other geotechnical engineering applications, for creating fluid-flow paths in low-permeability rock formations. Hydrofractures are typically produced by pressurizing a well with water to crack large blocks of rock underground and then injecting a "frac" fluid carrying a proppant to hold the fracture open. Hydrofracture techniques are primarily used to increase the productivity of marginal wells and may also be used as a means of disposing of waste fluids into low-permeability formations. Present hydrofracturing practices are "hit and miss" in nature with little knowledge of the complex processes at work or of the resulting changes in the rock formation; thus predictability and reproducibility are not available to those using the process such that its effectiveness and applicability can be relied upon.

At LBL we are developing instruments and methodologies for determining fracture orientation, fracture length, and the distribution of proppant in the fracture. Our primary efforts have been in the use of seismic techniques to monitor and locate seismic activity associated with rock failure and in the application of ultrasensitive magnetic detection methods to locate the distribution of highly magnetic proppant materials. These experimental studies have been carried out at many different scales—from the laboratory to massive hydraulic fractures in the field. Related studies are concerned with fracture mechanics and propagation, fluid-proppant flow, and an evaluation of improved electrical-electromagnetic techniques that can be used for fracture mapping.

(4) Enhanced Oil Recovery (EOR) Techniques
(k\$ 250)

C. Radke
W. Somerton

This project is investigating two major impediments to improving the efficiency of oil recovery and thus has the following principal research thrusts:

Clays present in oil-producing formations have an important effect on the success or failure of an enhanced recovery operation. The large surface areas of clays and the usually high reactivity of these surfaces may lead to the loss of injected chemicals by adsorption exchange and/or dissolution. Disruption of the equilibrium of the rock and its contained fluids caused by injecting fluids of different chemical compositions may result in the release and migration of fines and their subsequent deposition in pore necks or other restrictions in the flow paths. Changes in surface characteristics of minerals may also result from contact with steam, possibly affecting both flow and displacement behavior. In light of these problems, the objectives of this research are to characterize typical reservoir formations that might be candidates for EOR as to structure and mineral content, to evaluate chemical-loss characteristics, to gain an understanding of the mechanisms, and to develop techniques for minimizing deleterious effects. Use of clay-stabilizing agents and materials that inhibit chemical loss for each type of reservoir rock is being investigated. The problems of steam-condensate/clay reactions in steam-injection operations and the role of clays in fuel deposition in the *in-situ* combustion process are also being investigated.

Recovery of acid oils with simple alkaline agents is economically attractive. However, two major impediments must be overcome. The efficiency of tertiary recovery must be increased by improving mobility control, and the amount of alkali loss by rock reactions must be reduced. The approach being investigated in this research is the use of inexpensive additives to the caustic that will improve oil recovery and provide a source of multivalent cations for suppressing alkaline silica dissolution. Replacement of polymer by less-expensive additives and the modeling of the processes occurring are also under investigation.

(5) Studies of Aquifer Contamination
(k\$ 250)

C.F. Tsang

Groundwater contamination as a consequence of half a century of indiscriminate dumping and spillage of toxic waste has become a major problem all over the U.S. Several important questions may be raised regarding aquifer restoration and contaminant cleanup procedures. Such questions include: (1) what are the optimal monitoring arrangements? (2) what are the most effective cleanup procedures? and (3) how to estimate the cost-benefit of cleanup for a given site?

Several complementary projects are addressing these issues and developing improved methodologies for understanding and predicting contaminant transport in groundwater systems. Existing codes are being modified for contaminant transport applications and will be validated by the data from field experiments and case-history studies. A compilation of analytical and numerical methods has been published as a Water Resources Monograph of the American Geophysical Union. Data from several specific sites are being analyzed in an evaluation of cleanup procedures. A report is being prepared to review key issues involved in a determination of the extent of contamination cleanup.

(6) Assessment of Nuclear Waste Isolation
(k\$ 1100)

H.A. Wollenberg, Jr.

In fulfilling its regulatory responsibilities relative to geologic repositories for nuclear waste, the Nuclear Regulatory Commission (NRC) must evaluate proposed site plans from the standpoints of validity of the technologies used, accuracy of measurement instruments and techniques, reliability of predictive computer models, and legitimacy of alternative isolation schemes. This is a comprehensive research program on geoscience problems of major concern to the NRC. The overall goal of this program is to establish a base of geoscience knowledge adequate to provide a scientific foundation for the related NRC functions and responsibilities.

Activities include fundamental geochemistry studies to develop: (1) basic data on rock-water/nucleide interactions, (2) computer codes for radionuclide migration prediction, and (3) standardized analytical techniques. Further research is focused on understanding the coupled thermomechanical-hydrological-geochemical processes that would occur in repository environments and developing appropriate numerical models for such dynamic and complex processes. Considerable effort is also devoted to documentation of the models and laboratory techniques for use nationally.

(7) Geologic Storage of Nuclear Wastes
(k\$ 750)

P.A. Witherspoon

This is a multidisciplinary effort studying several geoscience topics fundamental to the safe long-term storage of nuclear wastes in geologic environs. The studies are focused on understanding and predicting the physiochemical processes occurring between buried materials and the surrounding rock as well as the transport of any leached radionuclides through the geologic systems. Topical investigations include the development of numerical techniques for predicting radionuclide migration, modeling of fluid flow through complex fracture-porous rock systems, and development of methods to measure the *in-situ* characteristics of rock masses. These studies furnish information fundamental to designing repository containments and measuring the long-term performance of storage sites. Additionally, engineering studies address the geologic questions central to repository development at specific sites and, in conjunction with DOE management, construct site-testing plans to clarify geotechnical engineering problems.

ENGINEERING AND TECHNICAL SERVICES DIVISION**W.D. Hartsough, Associate Director**

- (1) Heavy Nuclei Collection on the Long Duration Exposure Facility (LDEF) Mission II: Research, Design, Development, and Testing of Special Hardware (k\$ 2,600)**

D.T. Scalise

The objective of the LDEF Mission II—Heavy Nuclei Collection (HNC) is to obtain a statistically significant sample of actinide nuclei (approximately 35 events) resolved to within 1/4 charge. Actinide nuclei are rare; thus the HNC requires a product of detector area and exposure time of approximately 80-meter² years to collect tracks from 35 actinide nuclei. Limited tradeoffs are possible between detector area and the exposure time (up to 2.5 years maximum).

The detectors will be arrayed on the surface of a cylindrical satellite that will orbit the earth every 90 minutes at an altitude of 200 miles for 2.0 to 2.5 years. The LDEF satellite will be launched on the Space Shuttle in November 1986. After 2 years, the LDEF satellite will be retrieved from space by the Space Shuttle and returned to earth so that the collected actinide tracks can be analyzed.

There are a number of state-of-the-art engineering challenges in the LBL portion of this program, including the following:

1. The dynamic loading environment in the LDEF satellite is very severe (e.g., accelerations of 16.5 g at 20 Hz).
2. The personal safety of the astronauts and the prevention of damage to the Space Shuttle require that extraordinary engineering measures be taken to provide the necessary quality assurance, structural integrity, and reliability.
3. A novel Event Thermometer (ET) is required. The temperature of the detector stack at the time a track is produced must be known to achieve the 1/4-charge resolution for the actinide that produced the track. Thus the ET must be extremely reliable throughout the 2.5-year period in space. It must be capable of recording the temperature under the following conditions.
 - a) Temperature measurements may be required at any physical location point in the 45 detector stacks (each with 0.7-meter² exposure surface).
 - b) Temperature measurements may be required at 35 randomly occurring instants during the 2.5-year period when the actinide tracks are produced. Thus, except for a few seconds during the 2.5 years, the ET takes no measurements, but it must be ready to instantly record the temperature during the transit of each of the 35 actinide nuclei.
 - c) Temperature measurements should not require electrical power.

This ET is now undergoing research, design, and development.

(2) LBL/Bay Area Rapid Transit (BART) Program
(k\$ 5,660)

D.T. Scalise
D.J. Rondeau

Throughout a nine-year period (1974–1983), LBL lent its expertise in advanced technology toward solution of high-technology frontier problems facing BART. LBL scientists and engineers worked closely with BART engineers and staff to find solutions to many important equipment reliability, safety, and computer-system technical problems.

The LBL/BART program focused attention on two basic systems crucial to BART operation.

1. The Automatic Train Control (ATC) System.

This consists of two important subsystems.

- a) The Automatic Train Detection subsystem includes the 1,500 wayside track circuits along the 75 miles of BART tracks. The function of these track circuits is to detect the presence of a train within a track circuit's boundaries and to prevent the entrance of a following train until the first train has left the track circuit.
- b) The Automatic Train Operation (ATO) subsystem includes control equipment on board the train. The function of the ATO is to control the train motor, brakes, and open/close door operations.

2. The Central Computer Train Supervisor (CCTS) System.

The CCTS system includes the central train control room and equipment located at Lake Merritt that supervises the flow of trains to smooth out perturbations when equipment failures occur.

Poor equipment performance and reliability in the ATC system and the limited capacity and obsolescence of the CCTS system represented critical technological phases of BART's history.

**(3) Ten-Meter Telescope (TMT): Research, Design,
Development, and Testing of Special Equipment**
(k\$ 1,200)

D.T. Scalise
G. Gabor

The TMT project is a long-range endeavor of the University of California and the California Institute of Technology. It is based on a novel concept conceived and developed over several years by project scientist Jerry Nelson for an economical segmented-mirror telescope design consisting of 36 hexagonal segments moving in unison within extremely close tolerances. The Technical Demonstration (TD) is only one phase of the long-range TMT project.

The objectives of the TD can be divided into two phases:

1. Proof of Principle Without Optical Quality.

In this phase, the desired Control Loop performance is derived from the calculated worst-case wind-force perturbations. For a 1.0-Hz, 200-nm amplitude perturbation on a mirror segment, the automatic control system must reduce the amplitude to 20 nm.

2. Proof of Principle With Optical Quality.

One goal is the reduction of warping errors of up to 500 nm during fabrication to less than 50 nm by a dewarping harness.

Another task has been to design and build a new whiffle tree with flexible-pivot joints to remove low-frequency resonances in the passive support system.

- (4) **Tokamak Fusion Test Reactor (TFTR)
Neutral-Beam Systems: Research, Design,
Development, and Testing of Special Equipment**
(k\$ 950)

D.T. Scalise
J. Haughian

LBL is providing assistance to the Princeton Plasma Physics Laboratory as follows:

1. By fabricating special research equipment that cannot be obtained commercially.
2. By collaborating with TFTR engineers in the engineering research, design, development, and testing of other special equipment needed for the TFTR Neutral-Beam System.

Examples of special equipment that required LBL engineering research, design, development, and testing assistance include:

1. Flexible transmission lines to the TFTR neutral-beam ion sources.
2. Magnetic chamber extension of the ion source.
3. Pressure isolator plates for the flexible transmission lines.

- (5) **Two-Phase Critical Flow Reactor Safety Research**
(k\$ 70)

V. Schrock

The objective of this project is to perform experiments and provide a validated mathematical model for critical flow through small breaks located in horizontal pipes. This project is funded by the U.S. Nuclear Regulatory Commission.

Model development tasks have been as follows:

1. Develop a new theoretical model for critical flow using test data from existing programs.
2. Test and validate the new model using data from the Idaho National Engineering Laboratory and French experiments on critical flows through small breaks in horizontal pipes.
3. Issue a comprehensive final report.

It is expected that this project will be completed in FY 1985 at an additional cost of k\$ 50.

- (6) **Methodology of Information Generation**
(k\$ 200)

J.D. Lawrence
G. Haire

The Information Methodology Research Project (IMRP) is developing a system to provide computer-assisted aids to document editing and indexing for the Energy Information Data Base of the DOE's Office of Scientific and Technical Information. The goal is to provide more efficient processing of documents and document surrogates (citations) by using interactive computer techniques. The system draws on automatic indexing techniques but includes the indexer as an integral element of the system; the indexer is the decision-maker, while the computer provides "clerical" support.

(7) Atomic and Molecular Detection
(k\$ 107)

T. Hadeishi

Accurate, sensitive, and highly selective detectors are required to monitor emissions, effluent streams, and ambient air and water. This project uses gaseous discharge sources to produce light, modified by application of magnetic fields, to measure absorption due to specific molecules in samples and, thereby, to detect and quantify the concentrations of the species.

Three basic approaches are being studied:

1. Atomic species are monitored using the differential absorption of Zeeman components of emission lines. By tuning one component to an absorption feature while the other measures background (smoke), an accurate determination becomes possible (Zeeman absorption spectroscopy).
2. A similar technique can be used for molecules (TALMS—Tunable Atomic-Line Molecular Spectroscopy).
3. Using several atomic-line pairs that coincide with spectral regions of high- and low-molecular absorption, high-sensitivity simultaneous measurement of several molecules can be made (ALMS—Atomic-Line Molecular Spectroscopy).

(8) Application of Atomic Absorption to Gasifiers

T. Hadeishi

B. Loo

(k\$ 150)

A new measurement technique, atomic-line molecular spectroscopy (ALMS), has been demonstrated to be capable of simultaneous detection of several compounds in the high-temperature, high-pressure environment that typically exists in a gasifier. Another technique that is a few years older, TALMS (tunable atomic-line molecular spectroscopy), has been tested for several compounds that exist in combustor gas streams. The approach will be to adapt both ALMS and TALMS to *in-situ* measurement of the composition of gas streams in combustion and conversion processes.

The development of monitors based on these concepts results in higher-efficiency conversion and combustion processes while minimizing corrosion and reducing emission of pollutants.

(9) Physical Methods for Detection of Short-Lived Gaseous Species
(k\$ 145)

B. Leskovar

W.F. Kolbe

This project is designed to develop methods of detecting short-lived transient gaseous species of interest in atmospheric chemistry and in energy-production processes. The program is based primarily on using millimeter-wave rotational-spectroscopic methods for the characterization of certain molecules. Studies have shown that moving to higher millimeter-wave frequencies than traditionally used in microwave spectroscopy should yield a substantial increase in sensitivity, and the experimental program is designed to use state-of-the-art components to demonstrate the improvements. Early work focused on a 70-GHz instrument; this was followed by work on a 140-GHz instrument that has achieved sensitivities in the 100- to 200-ppb range with one-second time constant. Further work will focus on the use of Fourier transform methods to speed up analysis and on the development of a relatively portable instrument.

(10) Physical Methods for Chemical Analysis
(k\$ 165)

J.M. Jaklevic

The focus in this project is on the application of x-ray and charged-particle spectroscopy techniques to the analysis of samples that may have environmental or commercial origins. Much of the early work focused on x-ray fluorescence (XRF) techniques; this was complemented by work on x-ray diffraction methods using multielement detectors to speed up the analysis for chemical species. The virtues of the intense narrow-line x-ray sources at synchrotron light facilities have been explored using both the EXAFS (extended x-ray fine structure) and more conventional XRF techniques. Charged-particle methods are being developed and used for depth profiling of sample surfaces (such as semiconductors) of interest to industry.

(11) Semiconductor Radiation Detector Technology
(k\$ 360)

F.S. Goulding
B. Loo
E.E. Haller

This project is designed to develop the technology of radiation detectors with emphasis on semiconductor and other solid-state detectors. The work includes basic detector material studies, development of new types of detectors, and specialized electronic signal-processing techniques. The foundation of modern spectroscopy using semiconductor detectors has been laid by this project. Recent work has focused on native defects in germanium and silicon and on defects produced by radiation damage and the relationship of these defects and detector performance. Work is in progress on multielement silicon detectors and "on-chip" techniques for read-out from these detectors. Recent work has also resulted in some very significant developments in signal processing that improves both the energy resolution and counting-rate performance of spectrometers. The results produced by this project are rapidly used by a number of United States companies involved in materials, detector, and spectrometer-system development.

(12) Advanced Detector Systems
(k\$ 122)

F.S. Goulding
R.H. Pehl

This project is to develop the techniques, detectors, and hardware required for major areas of nuclear research performed at national and private laboratories in the United States. The results of this work are of great value to other areas of research, such as astrophysics and nuclear medicine.

Work on semiconductor detector telescopes continues with emphasis on thin contacts. Work has continued on multistrip silicon detectors having position resolution in the 10- to 100- μm range; these detectors may assume considerable importance in large systems used to detect the products of relativistic heavy-ion collisions. Interest in the neutrinoless double-beta decay of ^{76}Ge has led to work on ultralow-background germanium-detector systems. A specific experiment (with UC-Santa Barbara) has a goal of setting a limit of 10^{24} years on the decay half-life (equivalent to 1-eV neutrino mass).

(13) Double-Beta Decay in ^{76}Ge
(k\$ 130)

F.S. Goulding

Observation of the neutrinoless double-beta decay process occurring in ^{76}Ge (or other candidate nuclides) would represent the first observation of nonconservation of leptons in nuclear processes, and a measurement of the decay half-life would provide a determination of the mass of the Majorana neutrino. Working with a UC-Santa Barbara group, we are developing a germanium detector system (eight detectors, 7.5 kg of Ge) surrounded by active (NaI) and passive shields. The experiment is designed to set a half-life limit of $>10^{24}$ years in about one year of counting. This would establish a neutrino mass limit <1 eV. The system is being constructed

and installed in our low-background facility before being moved to an underground facility at the Oroville Dam site for the final experiments.

MATERIALS AND MOLECULAR RESEARCH DIVISION

N.E. Phillips, Associate Director

(1) Electrode Surface Chemistry (k\$ 200)

P.N. Ross

Commercialization of phosphoric acid fuel-cell technology requires a capital cost reduction and an extension of power-section life compared to currently available technology. Significant capital cost reduction can be achieved if an oxygen reduction catalyst can be developed that is catalytically more active than Pt supported on graphitized carbon black. Toward this end, extensive fundamental studies of Pt electrochemistry are being conducted to learn how Pt activity depends on temperature, acid anion, water concentration, and surface structure (morphology). Surface studies of gas-phase oxygen adsorption on small (20 Å) Pt clusters by x-ray photoemission spectroscopy have shown that very small Pt clusters are oxidized more readily than smooth Pt, thus causing a decline in oxygen reduction kinetics with crystallite size because of too strong an interaction with oxygen on the small clusters. These results suggest modification of the adsorptive properties of Pt by the substitution of ligands to the Pt coordination sphere, e.g. alloying, could result in enhanced Pt catalysts. The objective of the present research is to develop the physical and chemical understanding of oxygen-platinum-ligand interaction necessary for the rational selection of alloying components. Fundamental studies of the alloy-electrolyte interface using modern surface-science techniques should provide the means to optimize the alloy ligand or to redirect the search for more active materials along the most rational paths. Alloying may have significant beneficial effects on electrode performance above and beyond effects on the oxygen-reduction kinetics, e.g., reduced Pt dissolution and surface-area loss. These additional alloying effects will also be studied at the atomic level, e.g., surface reconstruction, surface self-diffusion.

(2) Electrochemical Energy Storage (k\$ 1500)

R.H. Muller
C.W. Tobias
P.N. Ross
J.W. Evans
L.C. De Jonghe
J. Newman
E.J. Cairns*

*(Affiliation: Applied Science Division)

The overall aim of the program is to improve energy efficiency, lower capital cost, and increase materials yield of electrochemical-cell processes employed for the reversible conversion of energy in galvanic cells. These goals are pursued in nine partially interdependent projects. *Surface Morphology of Metals in Electrodeposition*: Role of electric-field and solution-side mass transport in the electrocrystallization of metals; mechanism of initiation, growth, and propagation of surface imperfections; development of surface textures. *Metal Couples in Nonaqueous Electrolytes*: Exploration of organic solvents for the efficient deposition and dissolution of reactive metals. *Engineering Analysis of Electrolytic Gas Evolution*: Characterization of the physical processes involved in the evolution of gases at electrodes, with emphasis on their effect on ohmic resistance and mass transport. *Surface Layers on Battery Materials*: Experimental characterization of surface layers on electrodes and new approaches to control their properties. *Analysis and Simulation of Electrochemical Systems*: Development of mathematical models to predict the behavior of electrochemical systems and to identify important process parameters; experimental verification of the models. *Electrode Kinetics and Electrocatalysis*: Oxygen reduction with new catalysts and carbon black corrosion during oxygen evolution. *Electrochemical Properties of Solid Electrolytes*: Electrochemical behavior of sodium beta and beta

alumina for use in the sodium sulfur cell at temperatures between 200°C and 400°C. *Battery Electrode Studies*: Processes in electrodes for aqueous and molten salt electrolyte systems. *Electrical and Electrochemical Behavior of Particulate Electrodes*: Electronic conduction and metal dissolution/deposition in particulate electrodes.

(3) Electrochemical Processes
(k\$ 123)

C.W. Tobias

This program is designed to advance the scientific foundations of electrochemical engineering and to broaden the range of useful applications of electrochemical transformations. Present emphasis is on exploring *novel methods for reducing mass transfer resistance* in high-rate applications, including electroforming of metals and electro-organic synthesis. The effects of fixed flow obstacles and suspended inert solid particles in flowing electrolytes on transport rates and current distribution are measured over broad ranges of process variables; theoretical models are advanced for the interpretation of mechanisms. *Nonaqueous ionizing solvents* are explored for potential use in ambient temperature electrosynthesis processes, e.g., in the extractive metallurgy and electroplating of reactive metals. Present emphasis is on the development of viable techniques for the removal of trace impurities in propylene carbonate to below 10 ppb, to improve solvent stability in presence of energetic oxidizing or reducing agents.

(4) Electrochemical Phase Boundaries
(k\$ 138)

R.H. Muller

The purpose of this work is to advance the understanding of boundary layers and thin films at electrochemical interfaces. Boundary layers control the chemical environment in which electrode processes take place and are often responsible for limiting the specific rate at which reactions can be conducted. Thin films and adsorbed layers on electrodes greatly affect the kinetics of electrode reactions, such as the electrodeposition and dissolution of metals, and control the chemical properties of most metals in liquid environments. New optical techniques for the observation of electrode surfaces in liquid media are developed and used. They include spectroscopic ellipsometry combined with light-scattering measurement, Auger spectroscopy, interferometry, thin-film interference, and Doppler velocimetry.

(5) Investigate New Fuel-Cell Electrolyte and Electrode Concepts
(k\$ 70 Est.)

P.N. Ross

Phosphoric acid is the electrolyte currently in use for commercial hydrogen-air cells. It is a relatively weak acid ($pK = 2.1$), and there is specific adsorption of phosphoric acid anions on Pt surfaces that probably interfere negatively with the oxygen reduction reaction at Pt electrodes. Trifluoromethane sulfonic acid (TFMSA) is a very strong acid, and specific adsorption of the anion on Pt in 0.1-molar TFMSA appears to be minimal as determined by recent measurements. Therefore, it is expected that oxygen reduction on Pt electrocatalysts in TFMSA would proceed at higher rates than in phosphoric acid. Technologically, the problem with TFMSA as a fuel-cell electrolyte is that in the concentrated form needed in practice, the acid wets the polytetrafluoroethylene (PTFE) hydrophobic bonding agent used in gas diffusion electrodes, causing a collapse of the three-phase interfacial structure. It is hypothesized that this wetting is because of the CF_3 -functional group, and that multibasic homologs of this acid, e.g., tetrafluoroethane-1,2-disulfonic acid (TFEDSA), would not wet PTFE. Another technological problem with TFMSA is its relatively high volatility at practical operating temperatures ($>100^\circ C$). It is felt that higher homologs of TFMSA would have a lower vapor pressure, so that multibasic higher homologs of TFMSA may have all the advantageous properties of this acid but with low volatility and with desired wetting properties. The object of this program is to study oxygen reduction on the family of perfluoroalkylsulfonic acids to determine whether or not the desirable characteristics of TFMSA are intrinsic to this class of organic compounds.

(6) Photochemistry of Materials in the Stratosphere
(k\$ 252)

H.S. Johnston

This project is equally interested in fundamental physical-chemical studies of small molecules and in obtaining useful atmospheric data. Laboratory studies are carried out to obtain optical cross sections, quantum yields, infrared line shapes and absolute intensities, pressure-broadening coefficients, information about microscopic states, and macroscopic rate coefficients for molecules and reactions currently important toward interpreting atmospheric observations. The experimental methods include visible and ultraviolet laser flash photolysis, laser resonance absorption, resonance fluorescence, and infrared diode lasers. Theoretical methods include some molecular quantum mechanics and some numerical atmospheric modeling. This research has applications to problems of atmospheric ozone, and recently it has become apparent that this field of research is applicable to the role of gases other than carbon dioxide on the "greenhouse effect."

(7) Selective Photochemistry
(k\$ 152)

C.B. Moore

The fundamental goals of this program are to understand the photophysics of selective excitation of molecules, the dynamics of energy transfer and specificity loss, and the chemical reactions of specifically excited states. For low levels of vibrational excitation in small molecules, chemical reaction rate constants are defined for each quantum state. For larger, more highly excited molecules, energy is usually transferred among vibrational modes more rapidly than chemical reactions occur. The nature of the energy states of molecules as a function of excitation energy and of molecular size and structure determines the intramolecular flow of energy. The possibilities for limitations upon selectivity in photochemical processes are determined by the time evolution of the combination of spectroscopic states excited by the photons. A complete understanding of unimolecular dynamics is sought by both the examination of spectra and the measurement of reaction rates. The rates and mechanisms of free-radical reactions are often best studied by flash-kinetic spectroscopy using lasers for thermal heating, photolyzing, and spectroscopic probing. A fundamental understanding of these reactions is sought to serve as a basis for modeling combustion processes. Radical-radical collisions can lead to complex formation. Consequently, reactions and energy transfers between radicals can be understood in terms of unimolecular reactions.

(8) Actinide Chemistry
(k\$ 1320)

N.M. Edelstein

The purpose of this project is to study actinide materials in order to provide the basic knowledge necessary for their safe and economic utilization in present and future technology. The program includes the preparation of new gaseous, liquid, and solid phases and studies of their physical and chemical properties. Techniques for characterization include x-ray diffraction, optical and vibrational spectroscopy, magnetic resonance, and magnetic susceptibility. Equilibrium and kinetic data for complex formation are measured. From these complementary studies, new insights into the structural and chemical principles of actinide compounds are obtained with which to design new synthetic schemes to produce new materials. A major aspect of the program is the design and synthesis of sequestering agents for actinide ions. These compounds are intended for use in the treatment of actinide poisoning and for possible application in the treatment of spent reactor fuels. Preparative, structural, and physical studies of new types of organoactinide, related organolanthanide, and new actinide inorganic complexes are continuing. Studies on optical spectra of free ions and actinide ions in crystals are being pursued in order to understand their electronic structure. Applications of new spectroscopic techniques for characterization of actinide species in solution are being undertaken.

**(9) In-Situ Investigations of Gas-Solid Reactions
by Electron Microscopy
(k\$ 108)**

J.W. Evans
K.H. Westmacott

This research project is concerned with the kinetics of reactions between gases and solids of relevance to materials technology. Of central interest is the role that microstructure plays in such reactions. For example, in reactions where a second solid phase is nucleated during the course of the reaction (examples are the reduction of iron oxide to iron or the oxidation of gallium arsenide), the sites for nucleation and the growth of the second phase are to be related to the presence (or absence) of such microstructural features as the microcracks, grain boundaries, and dislocations. The principal experimental tool in this investigation is an environmental cell located in the high-voltage transmission microscopes at Berkeley. Within this device the reaction between a gas and a solid can be observed at the full magnification offered by these powerful instruments. A substantial change in the program is envisioned for FY 1986. By that time the useful work that can be done with the present design of environmental cell will have tapered off. This cell is limited in its performance; at 50 torr of gases the maximum temperature is 600°C. This renders the cell useless for studying many important reactions that occur at significant rates only at higher temperatures (e.g., the oxidation of silicon, the attack of oxide ceramics by hydrogen, the formation of silicon nitride by nitriding of silicon). Somewhat higher temperatures can be achieved by minor modifications of the cell; however, to make this experimental technique applicable to the plethora of high-temperature reactions encountered in materials science, radical modifications and a major instrument development effort are required. The initiation of research using an environmental cell in a scanning microscope at Berkeley is also planned for FY 1986.

**(10) High-Temperature Reactions
(k\$ 345)**

A.W. Searcy

The central program objective is to deepen scientific understanding of the kinetics and thermodynamics of high-temperature reactions. Recent emphasis has been on endothermic decomposition reactions. A general theoretical framework for analysis of decomposition reaction kinetics was developed under this project. With this background, a systematic investigation has been conducted on the separate influences of temperature, product gas pressure, thermal-energy balance, particle size, sample size, and catalysts on decomposition rates and on the structure and properties of solid-reaction products. Transmission electron microscopy studies of prototype decomposition reactions will complete this phase of the program, and studies of the more complex reactions of the kind illustrated by $\text{BaCO}_3 + \text{TiO}_2 \rightarrow \text{BaTiO}_3 + \text{CO}_2$ are planned. A concurrent investigation of vapor transport through porous solids is being used to obtain quantitative data on high-temperature surface diffusion. Theoretical and experimental studies of surface thermodynamics, chemisorption, and surface-transport processes are receiving increased emphasis. An important objective of the surface studies is to develop a model for the kinetics of molecular exchange between regions of different bond energies in an equilibrium particle.

**(11) High-Temperature Thermodynamics
(k\$ 173)**

L. Brewer

High-temperature chemistry is characterized by the occurrence of unusual species and phases that are often unstable at conventional temperatures. Because of the difficulty of carrying out measurements under high-temperature conditions, it is important to design experiments to yield information that can be used with predictive models. In this manner, one can often calculate chemical behavior under conditions where measurements have not been made or would not be practical. Since 1943, the research of this program has led to development of successful models of predictive capability for the behavior of gases at high temperatures, of

refractory containment materials, and of many metallic systems. For many alloys, the understanding of the interactions is adequate to provide quantitative predictive models. As an example, in 1980, a tabulation of the thermodynamic properties and phases diagrams of one-hundred binary systems of molybdenum was published. The main thrust of the present research is aimed at providing quantitative predictive models for the strongly interacting alloys exhibiting generalized Lewis acid-base behavior. A variety of experimental methods are being used to characterize the thermodynamics of these systems.

(12) Photon-Assisted Surface Reactions, Materials, and Mechanisms
(k\$ 233)

G.A. Somorjai

This project explores photocatalyzed chemical reactions that take place at the solid-liquid interface. These reactions include the photodissociation of water (H_2O) to produce hydrogen and oxygen and the photon-assisted reactions of carbon dioxide (CO_2) and water to produce simple hydrocarbons (photosynthesis). The purpose of these studies is to explore the mechanism of photon-assisted surface reaction and then to establish the optimum conditions (of surface structure, composition, temperature, and reactant mixture) to maximize the rate of production of the desired chemicals (hydrogen and/or hydrocarbons). The materials that are being used include iron oxides, silicates, and oxides of tungsten and molybdenum.

(13) Physical Chemistry with Emphasis on Thermodynamic Properties
(k\$ 138)

K.S. Pitzer

The purpose of this program is the discovery and development of methods of calculation of thermodynamic and related properties of important chemical systems by use of quantum and statistical mechanics together with experimental measurements for key systems. Primary emphasis will be on ionized systems, electrolyte solutions, and plasmas. Systems consisting of fused salts mixed in any proportion with water are being studied experimentally and with semiempirical theory. Recent theoretical advances include treatments of the dielectric constant of H_2O , the thermodynamics of ionic solutions in H_2O above its critical temperature, and the critical properties of pure ionic fluids such as NaCl. Earlier advances yielded improved equations for electrolyte solutions that are now being applied to a wide variety of systems of industrial or geological interest, including geothermal brines. Current efforts also include relativistic quantum mechanical methods for the calculation of energies, bond distances, and other properties of the ground and excited states of molecules containing very heavy atoms where the conventional nonrelativistic methods are inadequate. Such results are important in evaluation of possible laser systems and for models of catalytic entities, including heavy atoms such as platinum.

(14) Molecular Interactions
(k\$ 300)

W.A. Lester, Jr.

This program is directed at extending fundamental knowledge of the interactions that govern the dynamics of energy transfer, reactive, and photodissociative molecular processes. The approach is based on the reliable description of the potential energy surfaces and coupling matrix elements needed in theoretical approaches for the evaluation of cross sections and rates. Emphasis is placed on the use of state-of-the-art Hartree-Fock (HF), multiconfiguration HF, and configuration interaction (CI) *ab initio* methods for the accurate description of molecular interactions. A variety of methods are used to describe collision dynamics. The electronic structure studies emphasize the determination of the critical geometries and energetics that govern reaction pathways and include the computation of global potential energy surfaces where appropriate. The dynamics studies include fully quantum mechanical approaches to rotational-vibrational energy transfer in molecules by collision and an adiabatic approach to single-photon photodissociation of small polyatomic molecules and to chemical reaction. A

novel method that solves the Schrödinger equation stochastically is also being studied to ascertain its usefulness for determining the energy and other molecular properties.

(15) Theory of Atomic and Molecular Collision Processes
(k\$ 157)

W.H. Miller

This research is primarily involved with the development of theoretical methods and models for describing atomic and molecular collision processes. Specific topics of interest include the theory of inelastic and reactive scattering, collision processes involving electronically excited atoms or molecules, collisional ionization phenomena, statistical theories of chemical reactions, scattering of atoms and molecules from surfaces, and the interactions of molecular systems with high-power laser radiation. Much of this research is involved with the development and application of a general semiclassical mechanics that allows one to combine classical mechanics and quantum mechanics in a correct and useful manner. This has been extremely successful in providing an understanding of the various quantum effects that are seen in molecular phenomena, and it also often provides simpler computational methods for carrying out quantitative calculations. Certain research topics are more amenable to a completely quantum mechanical approach, and these sorts of theoretical techniques are also used. The ability to understand—and thus to model and to predict—chemical kinetics phenomena in the gas phase has widespread practical importance in a number of different areas. Among these are atmospheric chemistry and physics, interactions of molecules with strong laser fields, and energy transfer and chemical reactions in flames and combustion.

(16) Crossed Molecular Beams
(k\$ 648)

Y.T. Lee

The major thrusts of this research project are to elucidate detailed dynamics of simple elementary reactions that are theoretically important and to use the molecular-beams method to unravel the mechanisms of complex chemical reactions or photochemical processes that play an important role in many macroscopic processes. Molecular beams of reactants are used to study individual encounters between molecules or to monitor photodissociation events in a collision-free environment. Most of the information is derived from measurement of the product fragment energy and angular distributions using a unique molecular-beam apparatus designed for these purposes. Recent activities are centered on the direct probing of transition states of the $F + H_2$ reaction through the experimental observation of quantum mechanical resonance phenomena; the mechanisms of elementary chemical reactions involving oxygen atoms with unsaturated hydrocarbons; the dynamics of chemical reactions of electrochemically excited atoms; the primary photochemical processes of polyatomic molecules, radicals, and ions; the intramolecular energy transfer of chemically activated and locally excited molecules using overtone excitation processes; and the interaction potential of open-shell atoms with rare-gas atoms.

(17) Atomic Physics
(k\$ 245)

R. Marrus

The MMRD atomic physics group is concerned with a broad-ranging experimental study of collisions and spectroscopy in simple atomic systems. Particular emphasis is placed on those processes pertinent to controlled-thermonuclear-reaction devices and processes important to fundamental physical laws. Examples of such studies are (1) electron capture by low-energy multicharged ions; (2) x-ray spectroscopy of helium-like, lithium-like, and beryllium-like ions of high Z ; (3) parity violation in heavy atoms predicted by unified theories of weak and electromagnetic interactions; (4) charge capture and loss by fast multicharged atoms in solid and gas targets; and (5) study of quantum electrodynamic effects and relativistic effects in hydrogenic and helium-like uranium. These studies take advantage of unique facilities developed within the group or available at LBL. Examples of such facilities are (1) the LBL SuperHILAC

and Bevalac that produce a wide range of heavy-ion beams at energies greater than other facilities in the world, (2) ion trapping techniques developed within the group (this has made possible the application of this technique to more highly ionized states that have heretofore been achieved), (3) narrow-band, high-power UV lasers developed in our group for studying parity violation in atomic systems. In addition, an electron-cyclotron resonance (ECR) source will be available for atomic physics research beginning in FY 1985.

(18) Formation of Oxyacids of Sulfur From SO_2
(k\$ 49)

R.E. Connick

The research is aimed at understanding the fundamental chemistry of sulfur species formed from sulfur dioxide in aqueous solution and the chemical reactions of these species. The chemistry of these systems is of particular importance in the problems associated with atmospheric pollution by sulfur dioxide and the resulting formation of acid rain. Recent research has focused on the kinetics of the exchange of oxygen atoms between bisulfite ions and water, using the nuclear magnetic resonance of oxygen-17 for following the reaction. The present results indicate a rate law consistent with exchange through formation of sulfur dioxide. The most intriguing finding is that there are two separate bisulfite species present, presumably the two isomers, which differ in the attachment of the proton to the oxygen or the sulfur. The latter species is about one sixth as abundant as the former and does not exchange oxygens with water at a significant rate. A secondary and not closely related goal is to determine the factors controlling the rate of substitution reactions in the first coordination sphere of metal ions. Computer modeling of such systems is under way, and some results for a two-dimensional model have been published. The work will be extended to three dimensions using a more sophisticated model for water.

(19) Solid-State and Surface Reactions
(k\$ 410)

G.A. Somorjai

The research program is centered on studies of catalyzed surface reactions and investigations of the atomic structure of solid surfaces and adsorbed monolayers. The kinetics and mechanisms of catalytic surface reactions are studied using well-characterized crystal surfaces at low and high pressures by using a combination of surface science techniques. The materials that are mainly used in our studies are platinum, rhodium, iron and its compounds, rhenium, molybdenum, alkali metals, and bimetallic alloys. The adsorbates and reactants are mostly hydrocarbons, oxygen, hydrogen, and water. Part of the investigation is directed toward the atomic-scale understanding of the structure and catalytic behavior of metal surfaces. The other part of our studies is aimed at developing new catalysts that substitute for precious metals and exhibit high rates and selectivity.

(20) Catalytic Hydrogenation of Carbon Monoxide
(k\$ 166)
(k\$ 193)

G.A. Somorjai

A. T. Bell

The purpose of this program is to develop an understanding of the fundamental processes involved in catalytic conversion of carbon monoxide and hydrogen to gaseous and liquid fuels. Attention is focused on defining the factors that limit catalyst activity, selectivity, and resistance to poisoning and the relationship between catalyst composition/structure and performance. To meet these objectives, a variety of surface diagnostic techniques (LEED, AES, XPS, EELS, IRS, TPD) are used to characterize supported and unsupported catalysts before, during, and after reaction. The information thus obtained is combined with detailed studies of reaction kinetics to elucidate reaction mechanisms and the influence of modifications in catalyst composition and/or structure on the elementary reactions involved in carbon-monoxide hydrogenation.

(21) Synthetic and Phys'cal Chemistry
(k\$ 72)

W.L. Jolly

The main objective of this project is to determine the nature of the chemical bonding in transition-metal organometallic complexes related to catalytic systems. The experimental tool is gas-phase x-ray photoelectron spectroscopy, which provides atomic core-electron binding energies. The binding energies give information about the distribution of valence electron density and the nature of the chemical bonding in the molecules. By measuring the core-binding energies of appropriate transition metal compounds, it is possible to study the interaction of metal d-electrons with various ligands such as organic groups, carbonyl groups, and nitrosyl groups. One can identify and distinguish various modes of ligand-metal bonding that have analogs in the molecules chemisorbed on metal surfaces and in the intermediates of catalyzed organic reactions. Of particular interest are studies of metal cluster complexes, in which the ligand-metal interactions are very similar to those on metal surfaces.

(22) Surface Chemistry—Application of Coordination Principles
(k\$ 108)

E.L. Muetterties
(Deceased)

A definition of the coordination chemistry of transition-metal surfaces on a comparative basis with that of molecular metal complexes and molecular metal clusters is the research objective. Displacement reactions supplemented with diffraction and spectroscopic data will be used in the elucidation of structural, bonding, and chemical features of the nickel and platinum metal surfaces with chemisorbed molecules. Initial studies are focused on the chemisorption states of aromatic hydrocarbons, olefins, and acetylenes on nickel and platinum surfaces. Catalytic reactions of these molecules will be examined in an ultrahigh vacuum chamber equipped with an isolation cell. These catalytic reactions will be closely correlated with metal-cluster research so as to obtain a precise comparison between homogeneous and heterogeneous catalysis. Theoretical analyses, based on symmetry matching of energetically available metal surface orbitals with those of molecules and molecular fragments of hydrocarbon, have been developed for a further comparison with structural data.

**(23) Transition-Metal Catalyzed Conversion of CO, NO, H₂,
and Organic Molecules to Fuels and Petrochemicals**
(k\$ 155)

R.G. Bergman

The central objective of this program is the discovery of new chemical reactions between organic compounds and transition metals and the understanding of how these reactions work. Particular attention is given to transformations that involve the most fundamental bonding changes (e.g., formation and cleavage of bonds between carbon hydrogen, nitrogen, and oxygen) that occur in important large-scale transformations of organic compounds, such as those employed in industrial catalysis and stoichiometric organic synthesis. A recent discovery on this project was that a certain class of iridium complexes undergo oxidative addition into the carbon-hydrogen bonds of completely saturated hydrocarbons (alkanes). This is the first example of this long-sought C-H activation reaction, and research during the past year has been directed at understanding its scope and selectivity. Recently, methods for extending the iridium-based alkane activation chemistry to appropriately substituted rhodium complexes have been developed. Work is under way aimed at studying the properties of these different metal systems, understanding and comparing the mechanisms of the reactions, and developing methods for using this chemistry to convert alkanes into more useful, functionalized organic molecules.

(24) Structure and Properties of Transformations Interfaces
(k\$ 207)

R. Gronsky

Transformation interfaces include homophase boundaries, heterophase boundaries, and "free" surfaces at which solid-state reactions are either initiated or propagated. The goal of this research program is to determine the atomic configurations of such interfaces and to establish the relationship between their structure and relevant interfacial properties. Correlations have been found to date under this project between the segregation behavior, precipitation behavior, or deformation behavior of interfaces and their detailed defect structures. Experiments are carried out mainly by transmission electron microscopy, including energy dispersive x-ray and electron-energy-loss spectroscopies; results are correlated with theoretical predictions of interfacial phenomena. Effort is currently directed at extending these and other correlations to the atomic scale, enabling in the longer range the control of interfacial structure to enhance materials properties.

(25) Structure and Electrical Properties of Composite Materials
(k\$ 123)

R.H. Bragg

The purpose of this work is to understand how the properties of hard carbons and soft carbons are related to their structure. The latter undergo a structural transformation, i.e., graphitize, and become physically soft when heated above about 2000°C in inert atmosphere; whereas the former do not, even when heated above 3000°C. Soft carbons are fairly well understood, but basic knowledge concerning hard carbons is scant. In this project, glassy carbon (GC) has been studied as a model hard carbon because it is a chemically pure (i.e., elemental carbon), monolithic solid. The structural differences between the two classes have been found to be analogous to those between thermo-setting resins (hard) and thermoplastic resins (soft). Whereas soft carbons become semimetallic electrical conductors, hard carbons resemble amorphous semiconductors, and at low temperatures display one-dimensional conduction. The major unknown in carbon science now is the specific atomic mechanism(s) associated with the structural changes during graphitization. This work has led to the hypothesis that it is the decomposition of a graphite intercalation compound, and experiments to test this hypothesis, via direct synthesis, and related studies of the carbon-hydrogen system are being performed.

(26) Excitation in Solids
(k\$ 180)

C.D. Jeffries

The central objectives of this program are experimental studies of the onset of instabilities and pseudorandom behavior in solids, together with a detailed analysis and interpretation within the recently developed renormalization group theory of chaotic dynamics. This theory displays universality and predicts that similar and recognizable modes of behavior will be observed in a very broad class of nonlinear phenomena, e.g., turbulence in fluids; plasma instabilities; erratic behavior in nonlinear mechanical, electrical, and chemical systems; and various instabilities in semiconducting, magnetic, ferroelectric, and piezoelectric materials. The turbulence in solids usually has nonlinear microscopic origins; the chaotic dynamics can be viewed as a consequence of strongly driven elementary excited states. To facilitate direct comparison between observed behavior and theoretical models, specific experimental methods have been developed: bifurcation diagrams, phase space portraits, Poincaré sections, return maps, power spectral analysis, real-time and transient analysis, and probability density distributions. This program has concentrated to date on spin waves in ferrites and on semiconductors. A detailed and systematic study of the chaotic dynamics of driven p-n junctions in Si and Ge has revealed many universal patterns: periodic doubling bifurcations, onset of chaos, periodic windows, and intermittency. Spin-wave instabilities in ferrite spheres display period doubling, chaos, and intermittency and can be understood by two-dimensional quadratic map. Electron-hole plasma density waves in crystals of Ge exhibit a period-doubling route to chaos, periodic windows, and

quasiperiodicity. These results have a bearing on devices of high technological interest and on a very general class of nonlinear problems of practical importance.

(27) Theoretical Studies of the Electronic Properties of Solid Surfaces
(k\$ 75)

L.M. Failcov

The purpose of this program is to study properties of solid surfaces. In particular, the interest is in determining (1) structural properties of surfaces, namely, the organization and arrangement of atomic constituents at equilibrium; (2) constitutional properties of the surface, in particular, the segregation properties of alloys at the surface as a function of crystal structure, surface orientation, nominal chemical composition and temperature; (3) electronic structure of surfaces, in particular, electron states and electron densities in the neighborhood of the surface; (4) vibronic properties of surfaces; (5) magnetic properties of surface, both in magnetic solids (ferromagnetic and antiferromagnetic) and in nonmagnetic solids that may develop a magnetic surface layer; and (6) chemical—in particular the catalytic—properties of solids as they are related to basic physical properties (1)–(5). A variety of theoretical techniques and models to focus on the various properties (band-structure models, many-body electron physics, numerical relaxation techniques) are developed, but the emphasis is on physical aspects and their implication to experiments rather than techniques *per se*.

(28) Theoretical Solid-State Physics
(k\$ 105)

M.L. Cohen

The purpose of this research is to provide a microscopic theory of solids capable of explaining and predicting the physical properties of real materials. During the past few years a successful theory has been developed here. The theory is based on a quantum mechanical pseudopotential-local density-total energy approach, and the inputs are essentially only the atomic number and atomic mass of the constituent atoms making up a solid. Applications of the method have been made to surfaces, interfaces, optical properties, superconductivity, electronic structure, vibrational properties, static structural properties, high-pressure solid-phase transitions, transport, photoemission, chemisorption, and properties of molecules. Direct collaborations with experimental projects have been frequent, and the predictive power of the theoretical approach has been tested successfully.

(29) Surface, Chemisorption, and Theory of Solids
(k\$ 50)

S.G. Louie

The main objective is to provide a theoretical understanding for the observed properties of solids at a microscopic level. Recent studies include bulk crystals, solid surfaces, chemisorption systems, solid-solid interfaces, defects, and novel materials such as graphite intercalation compounds. *W* *a* *r* *e*-quantum mechanical methods have been developed to calculate the properties of these systems using only information from the constituent atoms as input. Comparisons with experiments show that these methods are highly accurate and of predictive power. Bulk materials research will focus on electronic, structural, and vibrational properties; crystal structure determination; solid-solid phase transformations; and defects in solids. Surface and interface research will focus on atomic and electronic structure; mechanisms for structural relaxations and reconstructions; energetics and vibrational spectra of adsorbed species; and analysis of photoemission and other experimental effects.

(30) Low-Temperature Properties of Materials
(k\$ 133)

N.E. Phillips

The major objective of this program is to obtain information that contributes to an understanding of the behavior of materials by the measurement of low-temperature properties of condensed-matter systems, particularly specific heats. There are numerous special cases in which specific heat data provide either a test of theoretical models or values of important parameters that could not otherwise be obtained. Much of the work is in the region below 1 K, where the temperature scale is not well defined and temperature-measuring techniques are not well established. Because accurate temperature determinations are important in obtaining useful heat capacity data, research is also conducted on methods of temperature measurement. An accurate temperature scale has been developed to 5 mK. Recent specific heat measurements include measurements on ^3He in the Fermi-liquid region that have established the correct values of parameters that are important to an understanding of the superfluid states; measurements on potassium, rubidium, and cesium to 0.1 K to test theoretical predictions of charge-density-wave effects; and measurements on CuMn in high-magnetic fields that have mapped out the theoretically predicted phase boundary of the spin-glass phase. Specific future objectives include an extension of the ^3He measurements to the superfluid phases, additional studies on spin glasses, and specific heat measurements at pressures to 20 kbar on mixed-valence compounds.

(31) Energy Transfer and Structural Studies of Molecules on Surfaces
(k\$ 105)

C.B. Harris

A proper description of the ways in which internal energy is transferred between molecules and surfaces through electromagnetic field interactions, particularly in the short distance regime, is crucial to the understanding of a wide variety of molecule-surface interactions including laser-induced photoionization and photochemistry at metal and semiconductor surfaces. In addition, surface-enhanced electromagnetic field interactions are fundamental to other phenomena such as surface Raman scattering and other nonlinear interactions. The long-range goals of this research are (1) to study and understand the general principles that underlie electronic and vibrational energy redistribution at metal surfaces and (2) to develop new laser techniques for characterizing metal surfaces and chemisorbed molecules in the visible and vibrational infrared portion of the electromagnetic spectrum.

(32) Photoelectron Spectroscopy
(k\$ 557)

D.A. Shirley

Electron spectroscopy: electronic structure of matter, as determined by photoelectron spectroscopy and related techniques. The electronic structure of gas-phase species, including high-temperature species, as determined by the use of pulsed synchrotron radiation, including absorption and time-of-flight photoelectron spectroscopy. Photoelectron angular distributions and correlation-state studies. Electronic structure of solids from angle-resolved, variable-energy photoemission. Atomic and electronic structure of surface-adsorbate systems. Photoelectron spectroscopy of metal clusters and other exotic species. Exploration and development of new experimental methods based on synchrotron radiation in the energy range 10–4000 eV, such as photoelectron diffraction, ARPEFS, and surface EXAFS.

(33) Potential Energy Surfaces for Chemical Reactions
(k\$ 214)

H.F. Schaefer, III

This research program has two goals, related yet distinct. The first goal is the development of new theoretical and/or computational methods for the description of "what electrons are doing in molecules," to use the words of Robert S. Mulliken. Specifically, the single outstanding problem in the field is the correlation problem, that of formulating models for going beyond the single-particle or Hartree-Fock approximation. The second goal of our research is to apply these theoretical methods to significant problems of broad chemical interest. Currently, two areas are of special interest: (1) model theoretical studies of chemisorption, metal clusters, and organometallic species and (2) potential energy surfaces that govern gas-phase chemical reactions. Research in the former area is ultimately aimed at a truly molecular understanding of catalysis, a subject pertinent to future energy requirements but sometimes approached by trial-and-error methods. In the latter area our research sometimes tends toward molecules potentially important in interstellar space, atmospheric chemistry, and the development of high-power laser systems. It is to be emphasized that in recent years theoretical chemistry has become a significant source not only of broad generalities but also of specific predictions concerning molecular systems that may be very important but inaccessible to experiment.

(34) High-Energy Oxidizers and Delocalized-Electron Solids
(k\$ 238)

N. Bartlett

The main aim of this program is the synthesis and characterization of new materials. The synthetic work tests models and theories that correlate physical properties (such as electrical conductivity) with chemical composition and structure. Present emphasis is on the study of two-dimensional extended atomic networks such as those derived from graphite, layer-form boron nitride, and their relatives. Electron-oxidation of such materials (with accompanying intercalation to form salts) generates durable and conductive materials (some better than aluminium). Chemical, stoichiometric, and structural requirements for the best conductivity are being defined. The layered materials can often be oxidized (and intercalated) electrochemically, the process also being reversible. Thus graphite may be reversibly converted by electrochemical means to a graphite fluoride of approximate composition $C_{2.5}F$. This novel material, which could be imported as a high-energy electrode, possesses a π -electron system that appears to be similar to that in pristine graphite. Physical and chemical studies are being applied to this and related materials to determine the structure and bonding changes that accompany the oxidation and reduction. Salts that are either proton conductors or fluoride ion conductors, but not metallic, and that are resistant to oxidation are being sought as solid electrolytes for use with the metallic layer-material salts.

(35) Quantum Monte Carlo for Molecular Studies
(k\$ 30 Est.)W.A. Lester, Jr.
P.J. Reynolds

An alternative to the conventional theoretical techniques for molecular studies will be undertaken. The approach is the quantum Monte Carlo method, which was developed and used primarily in nuclear and condensed-matter physics. In this approach, the many-body Schrödinger equation is re-interpreted as a diffusion equation. Simulation of the appropriate random-walk process allows one to calculate expectation values of molecular properties. In principle, these expectation values can be calculated exactly, subject only to statistical errors. In studies of small molecules (H_2 , LiH , Li_2 , and H_2O), the singlet-triplet energy gap in CH_2 , and the classical barrier height for the $H + H_2$ exchange reaction, we have used a simple but accurate approximation to ease the treatment of Fermi statistics. In that approximation, the calculated total energy remains an upper bound to the true energy. How good the bound is, as well as the magnitude of the statistical error, depends on the quality of an "importance function" that guides the diffusion into more probable regions of phase space. Yet, we have obtained

even the relatively simple importance functions from 75–100% of the correlation energy of the above-mentioned molecules and systems. We propose to continue this work and extend it in several directions. Among other things, we hope to further improve the accuracy of the method, to obtain excited-state properties, to calculate potential energy surfaces, and to remove the Born-Oppenheimer approximation in certain applications.

(36) Mechanical Properties of Ceramics
(k\$ 301)

A.G. Evans

This project is concerned with the mechanical reliability of ceramics at high temperatures. The principal research topics entail the development of predictive capabilities for the high-temperature failure of ceramics and for microstructure/defect development during sintering. Elevated-temperature failure studies are concerned with the initiation, growth, and coalescence of cracks during creep. Experimental measurements are being correlated with theoretical models containing the dominant microstructural variables. Sintering studies are examining the processes that dictate the presence of retained porosity and defects during solid-state and liquid-phase sintering.

(37) Interfaces and Ceramic Microstructures
(k\$ 10)

J.A. Pask

Program includes: kinetics and mechanisms of solid-state reactions, nucleation and growth phenomena, and distribution of phases in multiphase ceramic systems whose principal phase constituents are within the $\text{Al}_2\text{O}_3\text{-SiO}_2$ system; thermodynamic considerations of sintering with a liquid phase; mechanisms of corrosion of ceramic materials; and thermodynamics and kinetics of electrochemical reactions at glass-metal interfaces.

(38) Chemical Properties and Processing of Refractory Ceramics
(k\$ 247)

L.C. De Jonghe

The objective of this work is to study the reactions at ceramic/metal interfaces and their effect on the physical properties of such interfaces. Two different reaction types are considered: gaseous reduction of transition metal oxides and subscale oxidation of Ni/ZrO_2 interfaces. Metal oxides such as CoO are reduced with CO/CO_2 or $\text{H}_2/\text{H}_2\text{O}$ mixtures, and the effects of catalytic inhibition by sulfur on the product morphology are studied. The micromorphological development of an oxide layer at the Ni/ZrO_2 interface is studied as a function of the alloying elements contained in the ZrO_2 . Thermogravimetric analysis and electron microscope methods are applied to characterize the reaction mechanisms. Acoustic emission detection during thermal cycling is used to assess the integrity of the metal/ceramic joint. Reactions in the solid state during densification in the $\text{CaO-Al}_2\text{O}_3$ system are also examined.

(39) Ceramic Interfaces
(k\$ 143)

A.M. Glaeser

Numerous properties of ceramics depend strongly upon the nature of the microstructure, necessitating control of the microstructural characteristics developed during processing. The present research program focuses on the development of an improved understanding of several processes that dictate the microstructural changes occurring during both materials fabrication and utilization. Thermodynamic and kinetic models are being developed that consider the modifying effect of dihedral angle on the morphological stability of continuous grain boundary phases, e.g., continuous pore channels present during sintering and continuous second phases in eutectic alloys and composites. The effect of solute additions, specifically MgO , on the nature of grain boundary migration in pore-free Al_2O_3 is being characterized. Previous work on grain boundary migration in lead is being reexamined in light of evidence suggesting that behavior

interpreted as indicating the occurrence of a grain boundary structure transformation may reflect a chemical transformation rather than a purely structural one. Procedures are being developed for the fabrication of oxide powders for use in an experimental examination of particle coarsening because of vapor phase transport. The recrystallization behavior of cold-pressed NaCl powder compact is being investigated with *in-situ* hot-stage observations of pore-grain boundary interactions planned.

(40) Structure-Property Relationships in Semiconductor Materials
(k\$ 345)

J. Washburn

The purpose of this research program is to advance the understanding of structural defects including the structure of interfaces in semiconductor materials. Particular emphasis is placed on interfaces and defects that are formed during processing steps used for state-of-the-art solid-state-device manufacture such as ion implantation, oxidation, and contact formation. This approach has also led to several areas of basic research: for example, a continuing series of experiments aimed at a more complete understanding of the mechanism of the crystalline-to-amorphous transformation during ion damage in silicon and gallium arsenide, an investigation of the detailed mechanisms of crystal growth into amorphous zones, and a study of the growth of Cu_2S layers on the surface of CdS. High-resolution lattice-imaging electron microscopy combined with computer simulation of the images has been shown to be a powerful tool for revealing and interpreting fine-scale defects and interface structures, particularly when used in conjunction with complementary observations on the same specimens such as Rutherford backscattering measurements, secondary ion mass spectroscopy, and electrical or optical measurements. The new atomic-resolution microscope promises to extend the limits of detection to even smaller defects, perhaps making possible more direct correlations between the presence of specific structural defects and their electrical effects.

(41) Experimental Solid-State Physics and Quantum Electronics
(k\$ 270)

Y.R. Shen

The main objective of this program is to further basic understanding of lasers and laser-related physics. Emphasis is on development of linear and nonlinear optical techniques for material studies and applications of these techniques to probe linear and nonlinear optical properties of gases, liquids, liquid crystals, and solids. For this purpose, both theoretical and experimental research on various aspects of light interaction with matter are being carried out. Newly developed techniques are being used to study current problems of interest: isotope separation, photochemistry, surface physics, and phase transitions. Nonlinear optical effects in matter not yet clearly understood are also being investigated.

(42) Time-Resolved Spectroscopies in Solids
(k\$ 100)

P.Y. Yu

Interactions between elementary excitations in condensed matters (e.g., electrons and phonons) occur in picoseconds (10^{-12} sec) or less. By using picosecond tunable laser pulses produced by modelocked dye lasers, these fast processes can be studied in real time and from these results the strength of these interactions can be determined. Current investigations involve the study of the properties of dense electron-hole plasma created by picosecond laser pulses in semiconductors by light scattering spectroscopies and time-resolved emission spectroscopy; trapping of free carriers at deep, nonradiative centers in crystalline or disordered semiconductors; and carrier relaxation mechanisms in crystalline and amorphous solids.

(43) Structural Materials and Weldments for High-Field Superconducting Magnets
(k\$ 150)

J.W. Morris, Jr.

The purpose of this work is the design and laboratory development of improved structural materials for the case and structural supports of high-field superconducting magnets. The research is motivated by the need for new alloys having suitable strength and toughness in welded structures in high magnetic fields at 4.2 K, to satisfy the structural materials needs for future generations of high-field superconducting magnets. The project has three tasks. First is the development of new ultrahigh strength ferritic alloys and weldments for magnet structural applications. Second is the development and testing of new austenitic Fe-Mn alloys that offer high strength and toughness at cryogenic temperatures. The third includes testing and analysis of the mechanical properties of current and potential structural alloys in high magnetic fields.

(44) Electron-Phonon Coupling and the Properties of Thin Films and Inhomogeneous Superconductors
(k\$ 61)

V.Z. Kresin

Properties of inhomogeneous superconductors will be studied. A tunneling junction is an example of an inhomogeneous system. There is also another important example. Many superconductors used in different applications contain heterogeneities that have a scale of the order of the coherence length. We will consider the thermodynamic properties of such systems and the effect of heterogeneity on T_c . Magnetic screening in proximity systems will be considered [in collaboration with Drs. S. Wolf and R. Simon (NVR)]. Electromagnetic properties of proximity systems such as the penetration depth will be studied. Particular attention will be given to systems of the PP S-Sm-S, where Sm is a semiconductor. The effect of localized states, resonant tunneling will be studied. Two-dimensional structural transitions, induced superconductivity, and Josephson tunneling in the presence of size quantization will be studied. The Ginzburg-Landau theory, describing the behavior of superconductors in an arbitrary magnetic field, has been developed in the approximation of weak electron-photon coupling. We will generalize this theory in order to describe the properties of superconductors with strong coupling. Direct coupling between electron-phonon interaction, phonon-spectrum, and the parameters of the Ginzburg-Landau theory will be established.

(45) Microstructure, Properties, Alloy Design: Inorganic Materials
(k\$ 612)

G. Thomas

This is a multicomponent, interdisciplinary program in physical metallurgy and ceramics involving fundamental quantitative studies of the structure-property relationships in technologically significant materials involved in energy and conservation. All tasks involve characterization of both structure and composition at the highest levels of spatial (transmission electron microscopy) and chemical (spectroscopy) resolutions in order to understand the complexities of structure-chemistry-processing-property relationships, without which alloy design is impossible. Specific tasks include:

1. Dual-phase ferrite-martensite steels for rod and wire, optimization of microstructure and processing, analytical studies of solute partitioning, fatigue (with Prof. R. Ritchie), and wear.
2. Martensitic and bainitic steels, fundamental studies of phase transitions, relation to wear; surface treatments (laser technology), grain boundary precipitation and effect of copper.
3. Magnetic materials; structure of audio recording tape, piezoelectric materials, rare-earth alloys.

Overall objectives are to design new materials or to more efficiently use existing materials with technology transfer to industrial practice without large capital investment and to realize material and energy conservation.

(46) Solid-State Phase-Transformation Mechanisms
(k\$ 207)

K.H. Westmacott

The purpose of this program is to obtain a detailed knowledge of the factors that govern phase changes and phase stability in order to facilitate first principle alloy design for specific service applications. The powerful, direct-observational methods afforded by advanced electron optical techniques, especially high-voltage and high-resolution electron microscopy, are employed to deduce the mechanisms whereby phase transformations occur. Since accommodation of a new phase of disparate size or structure must involve deformation, the relationship between lattice defects and precipitate phase growth is studied. This approach has been fruitful, and a developing crystallographic theory of precipitation is progressively being tested with a parallel experimental program. Simple model systems are treated initially and followed by studies on complex alloy systems of importance in energy-technology applications. The resulting knowledge will contribute to understanding alloy stability in hostile environments and the design of superior materials.

(47) Local Atomic Configurations in Solid Solutions
(k\$ 138)

D.R. de Fontaine

The present study concerns the fundamental investigation of ordering and phase separation in certain metallic alloys. Both theoretical and experimental aspects are considered for the three following topics: (1) atomic ordering being studied in systems exhibiting the phenomenon of long-period superstructure formation; (2) the theoretical end tool being primarily the newly developed cluster-variation method of statistical thermodynamics; and (3) the experimental tool being high-resolution electron microscopy. Phase separation will be studied in systems exhibiting partitioning of substitutional and interstitial alloying elements, such as alloy steels, the theoretical tool here being multicomponent nucleation theory and the experimental one being transmission electron microscopy with full analytical capabilities. The third project, a new one, concerns the interaction of magnetic and ionic ordering in AuFe alloys that exhibit the spin glass phenomenon. The theoretical tool is to be a modification of the cluster variation method, the experimental one that of high-resolution transmission electron microscopy and diffraction.

(48) Theoretical Problems in Alloy Design
(k\$ 567)

J.W. Morris, Jr.

This project is a multifaceted program of metallurgical research that is concerned with the science of alloy design. It has three objectives: to build the scientific foundation needed to approach the problem of alloy design in a systematic way, to develop systematic approaches, and to create new alloys that satisfy advanced energy needs. Specific research tasks include (1) theoretical research on phase transformations in solids and on the influence of microstructure on engineering properties; (2) experimental research on fundamental problems in metallurgy, including the control of microstructure through thermomechanical processing, the influence of microstructure on engineering properties, and the development of probative materials testing techniques; (3) the development of new structural alloys for advanced energy systems, a task which is now mainly concerned with the design of improved structural alloys for low-temperature use; (4) welding metallurgy, including the development of appropriate weld-filler metals and weld microstructures to maintain toughness in high-strength welded alloys; and (5) the development of improved superconducting wires for use in high-field superconducting magnets.

**(49) Environmentally Affected Crack Growth
in Engineering Materials**
(k\$ 296)

R.O. Ritchie

The objective of this program is to examine, from a combined continuum and micromechanistic points of view, the respective roles of mechanical, microstructural, and environmental factors involved in the subcritical monotonic and cyclic growth of flaws in engineering materials. Current emphasis is being devoted: (1) to defining the role of environment and microstructure on microscopic-crack closure mechanisms and their effect on subsequent near-threshold fatigue growth of long and short cracks in steels below 10–5 mm/cycle and for inert, gaseous, aqueous, and viscous environments; (2) to the modeling of crack *growth* toughness. Characterization of macroscopic growth rate behavior and microscopic failure mechanisms is being achieved through the use of fracture mechanics, microstructural and surface chemistry (e.g., Auger and ESCA) analysis, and detailed fractography. The aim of this work, based on the mechanistic understanding obtained, is that guidelines can be presented for the development of both improved failure prediction and improved alloy design of fracture-critical materials.

**(50) Studies of Materials Erosion in Coal Conversion
and Utilization Systems**
(k\$ 350)

A.V. Levy

The erosion of material surfaces by small solid particles carried in gas and liquid carriers is being investigated. The materials are tested over a range of conditions that simulate portions of the operating environments of containment surfaces in coal gasification, liquefaction, and fluidized-bed combustion processes. The effects of elevated temperature corrosion in combination with the erosion are studied to determine the mechanisms and rates of the combined surface-degradation modes. The fluid mechanics of two-phase flow in gases and liquids that result in erosive patterns in various geometry containments such as curved pipes is determined. The predictive models of the flow patterns will be combined with an analytical model of the erosion process to result in a means for predicting rates of erosion in curved pipes of the types used in process plants. The properties of materials that directly relate to erosion behavior and that are elements of the erosion model are determined and used in the model to predict erosion rates.

**(51) A Review of Unsolved Problems of Pressing Importance
in Fluid-Mechanics-Affected Erosion**
(k\$ 6)

J.A.C. Humphrey

This program includes: literature review of the "state of the art" of fluid-mechanics-affected erosion problems of practical importance; identification and tabulation of currently unsolved problems of pressing importance and with significant financial impact; examination of research methodologies that are experimental, analytical, and numerical; proposal for a tentative program of research addressing the most pressing issues revealed by the review.

(52) High-Temperature Oxidation and Corrosion of Materials
(k\$ 90)

N.E. Phillips

The primary objective of this program is to understand the criteria by which materials are able to withstand high-temperature corrosive attack and, in particular, the development of protective scales that minimize further interaction with the environment. Factors of major significance include: the initial development of the protective scale; and the transport of reactants in and through the scale; the scale's structure, morphology, and growth mode; the chemical integrity of the scale when exposed to corrosive sulfate deposits. The ultimate goal is to relate

mechanisms of behavior to the thermodynamic, diffusional, structural, and compositional parameters of the metal oxides, sulfides, and other phases involved and to develop both quantitative and predictive alloy corrosion models.

(53) Abrasive, Erosive, and Sliding Wear of Materials
(k\$ 108)

I. Finnie

Determination of the basic mechanisms of abrasive, erosive, and sliding wear. Identification of similarities and differences in different types of wear to allow development of simpler screening tests. Examination of material properties and microstructural features needed for optimum wear resistance. Development of quantitative methods for wear prediction for both single-phase and heterogeneous materials.

(54) Erosion of Brittle Solids
(k\$ 128)

A.G. Evans

This project is concerned with the development of a fundamental understanding of erosion and strength degradation of brittle coatings and layers subject to impact by solid particles. The principal research directions involve studies of the damage created by individual particles and of the erosion characteristics under multiple impact conditions. The residual stress in the coating and the adherence to the substrate are important variables in the investigation. Hence, techniques for ascertaining the magnitude of the residual stress and for characterizing adhesion are essential study topics. Predictions of material removal by spalling, after projectile impact, constitute the primary product of this investigation.

(55) Inhibitive Salts for Reducing High-Temperature Oxidation and Spallation
(k\$ 50)

N.E. Phillips
J. Stringer

It has been known for many years that the addition of small amounts of reactive elements to heat-resistant alloys produces a marked improvement in the alloy's behavior under cyclic oxidation conditions. More recently, it has been shown that fine dispersions of a wide range of stable oxides in the alloy have essentially the same effect. Metallic additions affect the growth rate and the possible mechanism of scale development and result in increased adhesion. However, oxide dispersions also affect the initial transient stage of oxidation, making it possible to develop a continuous protective scale (namely, Cr_2O_3 or Al_2O_3) at alloy Cr and Al levels below those required in the absence of a dispersed oxide. Thus, in general, oxide dispersions are better than metallic additions, although they are not as conveniently produced, requiring either a powder-metallurgy route or an impractical internal oxidation treatment. An alternative approach is to deposit the active element oxide as a surface coating, since it is probable that, even in true dispersion containing alloys, it is only the surface concentration that is important. A surface-coating technique also possesses the obvious advantage that it can be applied to large, complex, or inaccessible assemblies or components already in service. The idea of surface coatings of this type is not new; indeed it was included in the original patents of the rare-earth effect, which makes it very appropriate to examine the feasibility of using surface coatings of stable oxides as a means of improving resistance to scale spallation and oxidation.

(56) Catalytic Gasification of Graphite or Carbon
(k\$ 100)

H. Heinemann

This program is designed to look at the basic chemistry of the reaction of carbonaceous materials with water in the presence of catalysts to produce hydrocarbons and/or synthesis gas. Much of the work is being carried out with graphite as a carbon source to insure that hydrogen or hydrogen in hydrocarbons is derived from water. Relatively low temperatures are being

used to favor the equilibrium $C + 2H_2O \rightleftharpoons CH_4 + CO_2$, which is almost thermally neutral. Earlier work has shown that in the presence of KOH as catalyst, higher hydrocarbons up to C_6 can be formed. This raises the question whether hydrocarbons are a primary product and syngas a secondary one, formed by steam reforming. The formation of hydrocarbons is a stoichiometric reaction in which each H_2 in water reacts to form a phenolate and hydrocarbon: $5C + 4KOH \rightarrow 4COK + CH_4$. It has been shown by surface spectroscopy that phenolate is present, and it has been found that it can be decomposed over metal oxides to make the reaction truly catalytic: $4COK \xrightarrow{MeO_x} 2K_2O + 2C + 2CO$; $2K_2O + 2H_2O \rightarrow 4KOH$. Further work is directed toward combining flow reactor studies with ultrahigh-vacuum-surface studies to follow the mechanism, to find the best catalysts for phenolate decomposition, to measure and improve kinetics, and to study the effect of added gases such as CO or COS.

- (57) **Chemistry and Morphology of Coal Liquefaction:**
Hydrodenitrogenation—Novel Methods for Nitrogen Removal from
Polynuclear Nitrogen Containing Heteroaromatic Coal Compounds
 (k\$ 50)

H. Heinemann

The removal of nitrogen from complex matrices such as coal liquids is an extremely important area of study. We recently discovered that polynuclear heteroaromatic nitrogen compounds can be selectively reduced only in the nitrogen-containing ring. We now wish to focus on the aspects of carbon-nitrogen cleavage in the saturated nitrogen heterocyclic ring of model coal compounds in order to better understand how nitrogen can be removed without additional substantial use of hydrogen gas for that reaction to occur. A dual approach will be followed that provides fundamental information on the cleavage of carbon-nitrogen bonds using metal complexes of rhenium, iridium, rhodium, and ruthenium. The important coordination of metal complexes to saturated nitrogen compounds followed by oxidative addition to a methylene group, alpha to the nitrogen atom, will allow formation of metalla-azacyclopropanes. These compounds will be reacted with nucleophiles to hopefully afford carbon-nitrogen bond cleavage. The compounds will also be reacted under hydrogenation conditions to provide a similar carbon-nitrogen bond cleavage reaction. The second approach carried out simultaneously will use various zeolite catalysts with incorporated metal ions such as rhodium and ruthenium in addition to hydrogen donors such as long-chain hydrocarbons for catalytic cracking.

- (58) **Chemistry and Materials Problems in**
Energy Production Technologies
 (k\$ 296)

D.R. Olander

The goal of this program is to characterize the chemical and physical behavior of materials in the high-temperature, radiation environment of fission and fusion reactors. The materials of the uranium-based fuels and the zirconium-based cladding materials of light-water nuclear reactors are of principal interest. The processes and properties studied include rapid transient vaporization of fuel materials by laser-pulsing, high-temperature corrosion of zirconium by steam and the release of volatile fission products from irradiated UO_2 . Another aspect of the program involves molecular beam studies of the chemical kinetics of gas-solid reactions, including hydrogen atom reactions with silicon and its compounds and the etching of metals of halogens.

(59) Spectroscopy and Structures of Reactive Intermediates
(k\$ 129)

R.J. Saykally

The principal objective of this program is to study spectra, structures, and properties of elusive reaction intermediates that are of importance in combustion processes. Present emphasis is on the development of three powerful new spectroscopic techniques for detecting very low concentrations of such reactive intermediates. A far-infrared laser magnetic resonance (LMR) spectrometer employing selective UV photolytic generation of the reactive species is presently being tested; optimization of the experimental parameters for study of the hydroxyl radical has been accomplished. Extension of this approach for the study of important carbene species (HCOH , HCCN , CH_2) is in progress. A totally new laser spectroscopy experiment has been developed. Molecular Beam Laser Electronic Resonance (MBLER), in which ultracold (10–50 K) reactive molecules are generated in a supersonic beam inside the cavity of a far-infrared laser and rotational transitions are tuned into resonance with the laser with a large DC electric field, complements the capabilities of LMR for the study of reaction intermediates. The system is being tested on stable molecules (CH_3F , PH_3) and will be extended to prototype reactive intermediates (OH , CH , CH_2) in the near future. The first measurement of the dipole moment of methylene (CH_2) is anticipated. A tunable far-infrared laser has been designed and constructed. This system will be employed for the more general study of reactive intermediates that are difficult to access with LMR or MBLER experiments.

(60) Organometallic Chemistry of Coal Conversion
(k\$ 135)

K.P.C. Vollhardt

The basic program objective is to apply organometallic processes and techniques to the solution of problems concerned with the conversion of coal to liquid and gaseous fuels. The potential of novel organometallic systems such as catalysts and photostorage devices is being explored. A series of experiments on trinuclear biscarbyne clusters as potential models for surface mediated carbon-carbon and carbon-hydrogen bond making and bond breaking processes have been completed. This work has led to the discovery of novel transformations in the coordination sphere of transition metal clusters including carbyne-carbyne coupling and decoupling, chalcogen-induced degradation, and electrophilic substitution chemistry at the apical carbon. In addition, a novel, thermally reversible photochemical vinyl-hydrogen activation has been observed with potential in photochemical storage devices. A new method for constructing fulvalene complexes has allowed the exploitation of unprecedented binuclear chemistry of homo- and heteronuclear transition-metal derivatives. Several of these compounds have shown novel and distinct chemistry of relevance to catalysis and photochemical storage cycles. These systems are being investigated as potential models in heterogeneous Fischer-Tropsch polymerization and the activation of small molecules. The preparation and isolation of soluble, defined-molecular systems have allowed structural and mechanistic information to be assembled in unprecedented material.

(61) High-Pressure Phase Equilibria in Hydrocarbon-Water (Brine) Systems
(k\$ 153)

J.M. Prausnitz

Phase equilibria are required for efficient design of large-scale separation processes (e.g., distillation and extraction) in the chemical and related industries. In this context, "efficient" refers to optimum use of raw materials and to conservation of energy. Since the variety of technologically important fluid mixtures is extremely large, it is not possible to obtain all desired equilibria from experiment. Therefore, the objective of this research is the development of molecular thermodynamics for interpretation and correlation of selected phase-equilibrium data toward reliable general prediction of phase equilibria for engineering. The correlations are expressed through semitheoretical physico-chemical models in a form suitable

for computer-aided design. In this research, particular attention is given to those systems that are of primary interest in energy-related industries, especially those concerned with fossil fuels and fossil-fuel-water mixtures. Development of molecular thermodynamics calls for a combination of theoretical, computational, and experimental work. Further, it demands simultaneous awareness of progress in molecular science and of realistic requirements for engineering design.

(62) Enhanced-Fuel Capability of Marine Diesels
(k\$ 100)

A.V. Levy

We will demonstrate the ability to use lower-cost, blended fuels in marine diesel engines by the use of metallic- and ceramic-based coating and surface treatment systems applied to the surfaces of combustion zone components. The long-term, in-service endurance test and evaluation program will consist of two major phases. The first phase will evaluate the performance of selected metallic- and ceramic-based coating and surface treatment systems for a period of approximately 6,000 hours with the designated diesel engine(s) operating on No. 2 marine diesel fuel. The second phase will evaluate the performance of selected metallic- and ceramic-based coating and surface treatment systems for a period of 6,000 hours with designated diesel engine(s) operating on a blended fuel having a viscosity in the range of 200 to 400 SRI. The metallic- and ceramic-based coating and surface treatment systems may be tested on all of the following major combustion system components: valves, liners, rings, cylinder heads, pistons, and turbocharger compressor blades. Planned removals and/or inspections during each phase will be accomplished at predetermined intervals of approximately 1,500 hours. Throughout the program, combustion-system component-performance analyses will be performed.

(63) Selective Catalytic Hydrogenation of Polynuclear Heteroaromatic Nitrogen Compounds
(k\$ 20)

H. Heinemann

Within the objectives of this program, it has been shown that Wilkinson's catalyst as well as ruthenium analogues can selectively hydrogenate polynuclear heteroaromatic compounds such as quinoline, benzoquinoline, acridine, phenanthridine, etc., solely in the nitrogen containing ring. It has further been shown that it is possible to heterogenize such catalysts on DVB-PS beads as well as on silica without loss of selectivity and in some cases with increased activity. It has been demonstrated that aromatic sulfur compounds are not poisoning the reactions and that phenols may be promoters. The major objective at this time is to learn to split a nitrogen-carbon bond in the partially hydrogenated polynuclear aromatic so that ammonia can be removed without hydrogenating the entire molecule. This would result in a substantial reduction of hydrogen requirements and, in addition, the reaction could be carried out at much milder conditions than conventional hydrocracking, thus avoiding side reactions.

(64) National Center for Electron Microscopy
(k\$ 1380)

G. Thomas
R. Gronsky
K.H. Westmacott

Organization and operation of a national, user-oriented resource for electron microscopy. Maintenance, development, and application of specialized instrumentation including an Atomic Resolution Microscope (ARM) for ultrahigh-resolution imaging, a 1.5-MeV High Voltage Electron Microscope (HVEM) with capabilities for dynamic *in-situ* observations, analytical electron microscopes for microchemical analysis and support facilities for specimen preparation, image analysis, image simulation, and instrument development.

**(65) Collaborative Research by Transmission
Electron Microscopy (TEM)**
(k\$ 50)

N.E. Phillips

This program has been established to foster collaborative research between scientists with specialized skills in advanced techniques of TEM and scientists from other disciplines with projects requiring sophisticated microstructural characterization. Under the program, postdoctoral or experienced visiting electron microscopists spend up to one year at LBL using the unique instrumentation available at the National Center for Electron Microscopy (NCEM) in collaborative programs with MMRD investigators recommended for support by the NCEM Steering Committee.

(66) Far-Infrared Spectroscopy
(k\$ 230)

P.L. Richards

Improvements in infrared technology are making possible increases in the sensitivity of many types of infrared measurements. In this project, improved types of infrared detectors, mixers, and spectrometers are being developed. Improved infrared techniques are being used to do experiments in areas of fundamental and applied infrared physics where their impact is expected to be large. Developments of infrared technology include completion of a liquid-helium-cooled diffraction grating spectroscopy, fabrication and testing of ultrasensitive photoconductive detectors for the 50–500 μm wavelength range, improved fabrication techniques for bolometric detectors to improve their ultimate sensitivity, development of a new class of far-infrared dichroic beam dividers, and development of far-infrared harmonic generation as a spectroscopic source. Experiments in progress include measurements of the near-infrared absorption spectra of molecules chemically adsorbed on metal surfaces, measurements of the infrared spectra of one-dimensional conductors including charge-density wave systems and organic superconductors, and measurements of the infrared photoconductivity of impurities in semiconductors.

(67) Superconductivity, Superconducting Devices, and 1/f Noise
(k\$ 270)

J. Clarke

The Superconducting *QU*antum *I*nterference *D*evices (SQUIDS) are being developed and used in a wide variety of applications, including geophysical measurements, noise thermometry in the milliKelvin temperature range, nonequilibrium superconductivity, and the measurement of electrical noise. An ultralow noise SQUID amplifier has been operated at frequencies of up to 100 MHz and is being used to improve the sensitivity of nuclear magnetic resonance and quadrupole resonance measurements. SQUIDS are also being operated at temperatures down to 20 mK to study their ultimate noise limitations for such applications as transducers for gravity wave antennas. Novel experiments are being used to investigate macroscopic quantum tunneling in Josephson tunnel junctions at milliKelvin temperatures. The nonlinear dynamics of circuits containing a Josephson junction are being studied, with particular regard to the noise in such systems. A detailed study is being made of the excess noise induced in metal films by electron bombardment in an electron microscope. This type of measurement may produce a new technique for characterizing a defect concentration of metals.

(68) Nuclear Magnetic Resonance (NMR)
(k\$ 227)

A. Pines

The primary objectives of the nuclear magnetism program are to develop methods in magnetic resonance spectroscopy and to use them to study molecular behavior in condensed phases. This demands an understanding of the interaction of nuclear spins with each other, with other degrees of freedom such as molecular translations, vibrations, and rotations, and with external

radiation such as light or radio-frequency sources. Novel methods developed under the program include multiple quantum spectroscopy, high-resolution solid-state NMR and magic-angle spinning, zero-field NMR, pulsed-laser, nuclear double resonance, and nuclear magnetic-isotope separation. These methods are being applied to understand structure and dynamics at the molecular level in a number of materials including ferroelectrics, liquid crystals, polymers, organic crystals, and zeolites. Some molecular properties change upon light excitation, and laser-magnetic double resonance is being used to examine how these changes dictate the course of photochemical reactions. New methods of detection are being developed to increase the sensitivity of detection, in particular, using rapidly switched superconducting fields and Josephson junction devices such as SQUIDS (Superconducting *QU*antum *I*nterference *D*evices).

NUCLEAR SCIENCE DIVISION

E.K. Hyde, Associate Director (Acting)

(1) Heavy-Ion Physics Research
(k\$ 7,635)

E.K. Hyde

This project covers basic physics investigations with heavy ions at the Bevalac/ SuperHILAC complex and the 88-Inch Cyclotron. It supports developments in instrumentation, provides collaboration with visiting researchers, trains graduate students, and stimulates the development of accelerators and facilities.

Research at the Bevalac uses beams of ions up to ^{238}U at energies up to 2.1 GeV/nucleon to study the basic nuclear physics of interactions induced by relativistic heavy ions. Recent investigations have focused on reaction mechanisms and the properties of nuclei under extreme conditions of density and temperature, exploitation of the new heavy-ion beams, Čerenkov-detector studies of anomalous projectile fragments, and an evolving program to study direct lepton and dilepton production.

Experimental heavy-ion research at the 88-Inch Cyclotron focuses primarily on (1) investigations of heavy-ion reaction mechanisms (with particular emphasis on transfer reactions), (2) the study of exotic nuclei far from the valley of stability, (3) the spectroscopy of high-spin states of nuclei, (4) studies of collective motion in heavy-ion-induced reactions, and (5) searches for and studies of unusual transuranium isotopes and elements.

Experiments at the SuperHILAC use ions from ^{20}Ne to ^{238}U to investigate heavy-ion reaction mechanisms, nuclear structure, and atomic physics and to search for exotic elements and isotopes. Particular research is focused on understanding the energy and angular distribution of deep-inelastic reaction fragments, on half-life and g-factor measurements of high-spin states, and on the study of β -delayed proton emitters in the rare-earth region.

(2) 88-Inch Cyclotron Operations
(k\$ 2,100)

R. Stokstad
D. Clark
C. Lyneis

The 88-Inch Cyclotron is a variable energy isochronous cyclotron with spiral-sector focusing. The maximum energies of light particles are 57 MeV for protons, 70 MeV for deuterons, 140 MeV for α particles, and 145 MeV for ^3He . The energies of heavy ions are limited by magnetic-field strength to $160 Q^2/A$ MeV, where Q is the charge state of the ion and A the mass in amu. Intensities of the light ions are limited by deflector power dissipation, and heavy-ion intensities are limited by source intensity. Heavy ions with masses up to 40 are used in typical nuclear science experiments, with charge states up to Ar^{8+} . For special applications at low intensity the cyclotron has provided fully stripped ions up to O^{8+} , masses up to 197, and charge states up to Au^{14+} . At present the ion sources used on the cyclotron include filament arc sources for light ions, PIG (Penning ion gauge) sources for a very wide variety of heavy ions, and a polarized proton and deuteron source that uses axial injection. An ECR (electron cyclotron resonance) ion source that is under construction will increase the energy of most heavy-ion beams by a factor of 2 to 3.

This project operates, maintains, and improves the cyclotron and beam-transport facilities up to the experimental areas, maintains the building and shop facilities, and coordinates the use by LBL scientists, graduate students, and scientists from institutions other than LBL. The cyclotron was used by 154 scientists from 34 institutions during FY 1983. Beam was received by 72 experiments.

(3) Nuclear Theory
(k\$ 840)

N. Glendenning
M. Gyulassy
W.D. Myers
J. Randrup
W.J. Swiatecki

The work of the nuclear theory group continues to include a broad range of nuclear-, particle-, and astrophysical aspects, addressed by a variety of approaches and techniques. We have found it possible to sustain the momentum in the direction of relativistic nuclear physics and the quark-gluon plasma and to strengthen our effort in the astrophysical domain, while actually broadening our support to ongoing experiments at all of LBL's accelerators. For ultrarelativistic nuclear collisions the main questions addressed are whether sufficient concentrations of energy and baryons can be achieved to create a quark-gluon plasma and what are its decay modes. This effort includes analysis of cosmic-ray data, relativistic fluid dynamics and string model calculations, estimates of transport coefficients, and analysis of a variety of possible signatures. Research related to the Bevalac program is presently on global-event analysis and composite formation in connection with the new data suggesting collective nuclear flow for the first time. In the field of low-energy nuclear dynamics we have, in addition to extending existing calculations, derived an important new term in the equations of motion, essential for the understanding of damped nuclear reactions and related processes. The dynamics of the angular momentum accumulation during a damped reaction has been studied rather thoroughly. The theory for treating the subsequent disposition of angular momentum by sequential decays has also been developed. Confrontation with existing data has been made, and desirable new experiments suggested. Static nuclear properties continue to be studied using a range of approaches, including the Thomas-Fermi approximation and the Droplet Model. This has led to important insights into problems related to the equation of state of stellar matter during a supernova collapse and explosion.

(4) Low-Energy Physics Research
(k\$ 1,150)

J. Cerny

This project covers basic physics investigations with light ions (protons through ^4He , including polarized protons and deuterons) at the 88-Inch Cyclotron. In addition, it supports developments in instrumentation, provides collaboration with visiting researchers, trains graduate students, and stimulates the development of accelerators and facilities.

Studies of light nuclei far from stability use light-ion beams and the on-line mass-analysis system RAMA (recoil atom mass analyzer). Searches are conducted for nuclei near the proton and neutron drip lines that may decay by new or exotic radioactivities. Work has focused on studies of the newly discovered decay mode of beta-delayed two-proton radioactivity. Light-ion beams are also being used to investigate the advent of fission-like phenomena in deep-inelastic collisions. Spin-polarization effects in nuclear reactions are studied in collaboration with outside users, making use of the excellent polarized proton and deuteron beams from the 88-Inch Cyclotron. Experiments designed to test the basic symmetry properties of the nuclear interaction are in progress.

(5) Isotopes Project
(k\$ 370)

J. Dairiki

The Isotopes Project compiles and evaluates nuclear structure and decay data and develops compilation methodology. From 1940 to 1978 the Project's main objective was production of the *Table of Isotopes*. Since publication of the seventh (and last) edition in 1978, the group has coordinated its evaluation efforts with those of other data centers via the national and international nuclear data networks. The group is currently responsible for the evaluation

of mass chains $A = 167-194$. All evaluated data are entered into the international Evaluated Nuclear Structure Data File (ENSDF) and published in *Nuclear Data Sheets*.

In addition to the evaluation effort, the Isotopes Project will produce the *Radioactivity Handbook* for applied users of nuclear data. Recommended decay data will be taken from the current version of ENSDF without any updating; publication is planned in FY 1985. The group has also submitted a proposal for a complementary volume—the *Nuclear Structure Handbook*.

Promoting the science of nuclear data evaluation and providing assistance for the user community are also important aspects of the Project's role. Examples of activities in these areas are organization of the First Conference on Nuclear Structure Data Evaluation held at Asilomar October 27-30, 1981, and use of the DATATRIEVE data-base management system to make ENSDF data retrievable on-line. In addition to answering specific data requests, the Isotopes Project encourages general use of its extensive library, which contains comprehensive data files and major nuclear physics journals.

PHYSICS DIVISION

G.H. Trilling, Associate Director

(1) High-Energy Physics Research
(k\$ 8400)

G.H. Trilling

This program is concerned with experimental and theoretical research in high-energy physics. Experimental research is carried out using the particle accelerators at the Stanford Linear Accelerator Center (SLAC), the Fermi National Accelerator Laboratory (Fermilab), Tri-University Meson Facility (TRIUMF), and other laboratories. The broad purpose of this research is to perform experiments that will contribute significantly to the development of a fundamental theory of matter. The extensive planning, design, and implementation of these experiments are carried out at LBL, as are the data analysis and preparation for publication. The theoretical work is partly independent research in all aspects of particle theory and partly research motivated by or responding to the experimental program.

Part of the experimental work is directed toward full use of the Positron-Electron Project (PEP), the electron-positron colliding-beam facility at SLAC, through collaborative experiments using the Mark II detector (PEP-5) and the Time Projection Chamber (TPC) (PEP-4).

Most of the remaining experimental program is directed toward future exploitation of the 2-TeV $p\bar{p}$ facility at Fermilab (Tevatron I) and the 100-GeV e^+e^- linear collider at SLAC [Stanford Linear Collider (SLC)]. The Tevatron I effort consists of development and construction of parts of the Collider Detector Facility and D-zero detectors. The SLC program involves the construction of a new calorimeter as part of the upgrade of the MARK II detector for operation at 100 GeV.

(2) Positron-Electron Project (PEP)—Facilities Operation
(k\$ 700)

G.H. Trilling

This program is concerned with the operation of PEP-4, the Time Projection Chamber (TPC) facility installed in the Interaction Region 2 at PEP.

(3) High-Energy Technology
(k\$ 1900)

G.H. Trilling

The work on high-energy technology is devoted to research and development (R&D) for advanced detector systems both at LBL and other U.S. laboratories. LBL's unique capabilities in its electrical/electronic engineering and mechanical engineering departments permit LBL physicists to undertake extensive R&D efforts of ultimate benefit to the whole high-energy physics community, and beyond.

The experience and expertise developed in the course of creation of the Time Projection Chamber (TPC) in the Positron-Electron Project (PEP-4) are being applied to improvements to the present TPC, to R&D on high-pressure TPCs, and possibly to other TPC-related detectors. Other areas of detector development are very compact solid-state (large-coupled device) detectors, scintillating glasses, room-temperature liquids for hadronic calorimeters, highly segmented hadronic calorimeters, thin superconducting magnets, and drift and multiwire proportional counters with associated read-outs and electronics. Many of these R&D efforts have applications in industry and in research fields other than high-energy physics.

(4) Analytical and Numerical Methods
(k\$ 580)

A.J. Chorin
P. Colella
P. Concus
A. Fogelson
F.A. Grunbaum
O.H. Hald
A. Majda
J. Sethian

This program focuses on the areas of vortex dynamics and turbulence, high-resolution methods for hyperbolic equations, fronts and interfaces, reacting flows, capillarity phenomena, inverse problems, and numerical solutions of elliptic partial differential equations. A central goal is the construction of mathematically sound, computationally efficient, and physically realistic models that can lead to fundamental scientific understanding and can be used for engineering purposes. The vortex dynamics and high-resolution methods provide powerful and general techniques for solving the equations that arise in turbulent flow, multiphase displacement in porous media, and other areas. Coupled with additional techniques, they are an effective basis for attacking problems in reacting flows, such as combustion and flame propagation. The other topics of interest yield numerical and mathematical methods for attacking broad classes of problems including the reconstruction of images of objects from projection data of their transverse sections and the discontinuous behavior of capillary surfaces. Related new areas to be treated under the program are phase transition, liquid helium, and stochastic ordinary differential equations.

(5) Determination of the Atmospheric Carbon Dioxide Budget by Precise Measurements of the Oxygen-to-Nitrogen Molecular Ratio
(k\$ 175)

P. Tans

The rise in the atmospheric CO_2 concentration caused, at least in part, by the combustion of fossil fuels is expected to have a profound impact on the global climate. The credibility of current predictions of increases in atmospheric CO_2 is seriously impaired by the apparent imbalance in the present CO_2 budget. Very precise measurements of changes in the global atmospheric O_2/N_2 ratio in the course of a few years could provide the key to the solution of the "missing- CO_2 " problem.

An apparatus has been built that uses Raman scattering from a laser beam to make precise comparative measurements of the O_2/N_2 ratio in a sample and a standard. The scattering targets (air) are located inside the laser cavity. Interference filters match the spectral signatures of O_2/N_2 . Coupled choppers rotating at about 50 Hz interchange the signal from sample and standard. We have obtained the required stability in the comparison of intensities to about one part in a million. We are now measuring air samples from various places around the world to establish a series of precise reference values.

NAME INDEX

- Ainsworth, E.J. 43
 Alonso, J.R. 3
 Alpen, E.L. 44
 Amer, N. 19, 21
 Ames, B.N. 42
 Asaro, F. 23
 Attwood, D. 5

 Bartholomew, J.C. 65, 66, 68
 Bartlett, N. 96
 Bartley, J.C. 34
 Bassham, J.A. 69
 Bearden, A.J. 57
 Bell, A.T. 91
 Bergman, R.G. 92
 Berman, S. 14, 15
 Bissell, M.J. 39, 40
 Blanch, H. 7
 Bragg, R.H. 93
 Brecher, G. 28
 Brewer, L. 88
 Brown, N.J. 18, 20
 Budinger, T.F. 53, 54, 58

 Cairns, E.J. 7, 8, 85
 Calvin, M. 65, 67
 Castro, J.R. 48
 Cerny, J. 110
 Chan, D. 59
 Chang, S.G. 20, 22
 Chatterjee, A. 45, 50, 52
 Chorin, A.J. 114
 Clark, D. 109
 Clark, J.H. 67
 Clarke, J. 62, 106
 Clemons, G.K. 29, 38
 Cohen, M.L. 94
 Colella, P. 114
 Concus, P. 114
 Connick, R.E. 91
 Cooper, P.K. 31, 43
 Cooper, W.S. 2
 Cornacchia, M. 3
 Curtis, S.B. 46

 Dairiki, J. 110
 Daughton, C.G. 19
 De Fontaine, D.R. 100
 De Jonghe, L.C. 63, 85, 97
 Denn, M.M. 8, 62
 Derenzo, S.E. 53

 Durbin, P.W. 41

 Ebbe, S.N. 28, 29, 57
 Edelstein, N.M. 87
 Elioff, T. 5
 Esposito, M.S. 30, 31, 42
 Evans, A.G. 97, 102
 Evans, J.W. 85, 88

 Fabrikant, J.I. 44, 50
 Falicov, L.M. 94
 Finnie, I. 102
 Fish, R. 7
 Fogelson, A. 114
 Forte, T.M. 58

 Gabor, G. 80
 Glaeser, A.M. 97
 Glaeser, R.M. 54, 56
 Glendenning, N. 110
 Goodman, J.W. 27, 39
 Goth-Goldstein, R. 38, 39
 Goulding, F.S. 83
 Grimsrud, D. 15, 16, 17
 Gronsky, R. 93, 105
 Grunbaum, F.A. 114
 Gyulassy, M. 110

 Hadeishi, T. 82
 Haire, G. 81
 Hald, O.H. 114
 Hall, H.G. 35
 Haller, E.E. 61, 83
 Harris, C.B. 95
 Harris, J. 14
 Haughian, J. 81
 Hayes, T.L. 56
 Hearst, J.E. 66, 68
 Heinemann, H. 102, 103, 105
 Holmes, H. 73
 Hosoda, J. 32
 Huesman, R.H. 52
 Humphrey, J.A.C. 101
 Hunt, A. 10, 11
 Hyde, E.K. 109

 Jaklevic, J.M. 83
 Jeffries, C.D. 93
 Johnston, H.S. 87
 Jolly, W.L. 92

 Kammerud, R.C. 9
 Kaufman, A.N. 1, 5

- Keefe, D. 4
 Kim, S.-H. 66
 King, C.J. 9
 Klein, M.P. 65, 67
 Kolbe, W.F. 82
 Kresin, V.Z. 99
 Kunkel, W.B. 1, 2

 Lambertson, G. 3
 Lawrence, J.D. 81
 Lee, Y.T. 90
 Lemmon, R.M. 69
 Leskovar, B. 82
 Lester, W.A. Jr. 89, 96
 Levine, M. 24
 Levy, A.V. 101, 105
 Lindgren, F.T. 27
 Lippmann, M.J. 75
 Littlejohn, R.G. 1, 5
 Loo, B. 82, 83
 Louie, S.G. 94
 Lyman, J.T. 48, 49
 Lyneis, C. 109

 Maestre, M.F. 33
 Majda, A. 114
 Marrus, R. 90
 Martin, M.R. 9
 Marx, J. 3
 McCarthy, J. 72
 McEvilly, T.V. 75, 76
 Mehlhorn, R. 23
 Mcier, A. 14
 Merrill, D.W. 72
 Miller, W.H. 90
 Moore, C.B. 87
 Morris, J.W. Jr. 99, 100
 Morrison, H.F. 76
 Mortimer, R.K. 29, 30
 Muettterties, E.L. 92
 Muller, R.H. 85, 86
 Myers, W.D. 110

 Nero, A.V. 13, 16, 17
 Newman, J. 85
 Novakov, T. 18, 22

 Olander, D.R. 103
 Oppenheim, A.K. 21
 Orvos, J. 65, 67

 Packer, L. 11, 23
 Pagni, P. 22

 Parry, G. 34
 Pask, J.A. 97
 Pehl, R.H. 83
 Phillips, N.E. 95, 101, 102, 106
 Pimentel, G.C. 67
 Pincosy, P.A. 2
 Pines, A. 106
 Pitzer, K.S. 89
 Place, J.W. 9
 Prausnitz, J.M. 104
 Prosnitz, D. 3, 6
 Pyle, R.V. i, 2

 Quong, C. 73

 Radke, C. 76
 Randrup, J. 110
 Rapoport, H. 69
 Reynolds, P.J. 96
 Richards, P.L. 106
 Ritchie, R.O. 101
 Ritschard, R.L. 24
 Robben, F. 17, 19
 Rondeau, D.J. 80
 Rosen, H. 20
 Rosenfeld, A.H. 12
 Ross, P.N. 85, 86

 Sargent, T.W. 54, 55
 Sathaye, J. 25
 Sauer, K. 67
 Sawyer, R. 18
 Saykally, R.J. 104
 Scalise, D.T. 79, 80, 81
 Schaefer, H.F. III 96
 Schimmerling, W. 46, 48
 Schipper, L. 25
 Schlachter, A.S. 1
 Schooley, J.C. 37
 Schrock, V. 81
 Schwarz, R.I. 37
 Searcy, A.W. 88
 Selkowitz, S. 10, 15
 Selvin, S. 72
 Sessler, A.M. 3, 6
 Sethian, J. 114
 Shen, Y.R. 98
 Shirley, D.A. 95
 Shoshani, A. 71
 Smith, L. 3
 Somerton, W. 76
 Somorjai, G.A. 63, 89, 91
 Stampfer, M.R. 33, 35

Stokstad, R. 109
Stringer, J. 102
Sventek, J. 71
Swiatecki, W.J. 110

Tans, P. 114
Taylor, C. 3
Tenforde, T.S. 36
Thomas, G. 99, 105
Thomas, J.F. 19
Tien, C. 19
Tobias, C.A. 47
Tobias, C.W. 85, 86
Tomas, G. 105
Trilling, G.H. 113
Tsang, C.F. 77

Vella, M.C. 2
Vollhardt, K.P.C. 104

Wahlig, M. 9
Washburn, J. 98
Westmacott, K.H. 88, 100, 105
White, M.R. 36
Wilke, C. 7
Witherspoon, P.A. 77
Wollenberg, H.A., Jr. 77

Yano, Y. 51
Yourd, R. 5
Yu, P.Y. 98

SUBJECT INDEX

- accelerators 3, 4, 109, 110
 acid rain 91
 actinide chemistry 87
 actinides 41, 79
 active radicals 21
 aerosols 18, 20
 air conditioners 10
 air pollution 12, 13, 16-18, 20, 22, 36, 87, 91, 96
 alkaline earths 41
 alkanes 92
 alkylating agents 38, 39
 alkylation 43
 alloys 89, 99-102
 ALMS 82
 Alzheimer's disease 54, 55
 amine 9, 20, 66
 amino acids 11
 ammonia 9, 23, 105
 apolipoproteins 27
 appliances 13, 24, 25
 aquifers 77
 arctic region 20
 aromatic amines 20, 66
 aromatic hydrocarbons 34
 aromatics 92, 105
 Asclepias 65
 ASEAN countries 24
 astrophysics 110
 atherosclerosis 27, 28
 atmospheric chemistry 18, 22, 87, 91, 96
 atomic detection 82
 atomic physics 1, 90, 91
 Atomic Resolution Microscope (ARM) 105
 automotive engines 18

 bacteriorhodopsin 11
 ballasts 14, 15
 batteries 7, 85
 battery electrodes 8
 Bay Area Rapid Transit (BART) 80
 beam cooling 3
 beam injectors 1, 2
 benzo(a)pyrene (BaP) 33-35
 Bevalac 3, 4, 47, 48, 50, 51, 109, 110
 Bevatron 4
 biochemistry 69
 biomass 7, 23
 biomedical research 27-59, 65, 66
 biophysics 65, 66, 68
 blood 27-29, 39
 blood flow 54

 blue-green algae 23
 bone marrow 28, 37
 Bragg peak 44, 48, 50-52
 brain disorders 44, 45, 50, 51, 54, 55
 breast cancer 33-35
 brine 89, 104
 building materials 13
 buildings 9, 10, 12-17, 24, 25

 cancer 34, 39, 40, 42-50, 52
 carbides 63
 carbon 22, 93, 102-104
 carbon dioxide 20, 36, 114
 carbon monoxide 13, 16, 17, 91
 carbon particles 18, 20, 22
 carbon paths 69
 carbon-nitrogen bonds 103
 carcinogens 16, 31-35, 38-44, 56, 66
 cardiovascular flow 53, 58
 catalysts 11, 20, 63, 85, 86, 91, 92, 94, 96, 102-104
 catechols 41
 cell membrane proteins 54
 cells, biological 23, 28-31, 33-35, 37-40, 42-44, 46, 47, 56, 65, 66
 cells, energy 7, 8, 85, 86
 cellulose 7
 census data 72
 Center for X-Ray Optics 5
 central nervous system (CNS) 44, 50
 centrifugation 27
 ceramics 11, 63, 97, 99, 105
 chaotic dynamics 93
 charged-particle beams 44-50
 chelate catalyst 20
 chelating agents 41
 chemical complexation 9
 chemical oxygen demand 9
 chemisorption 92, 94, 96
 chillers 10
 chloroplasts 67
 chromatography 27
 chromosomes 33
 climate 20, 36, 37, 114
 coal conversion 9, 101-104
 coal-slurry diesel engine 17
 coatings 102, 105
 collaborative research 59
 collagens 35, 38
 colliders 3
 collision processes 90
 colloidal sols 11
 colloids 63

- combustion 18-22, 87, 101, 104, 105, 114
- combustion pollutants 17
- commercial buildings 12, 14, 15, 24, 25
- complexation 9
- composites 62
- Computerized Instrumented Residential Audit (CIRA) 12
- computers 71-73, 81
- condensate water 9
- conductivity 96
- cooling 9
- coordination chemistry 7
- corrosion 101
- crack growth 101
- crossed molecular beams 90
- crude oil 7
- crystals 61, 63
- cyanobacteria 23
- cyclotron, 88-inch 109, 110
- data bases 71-73, 81
- daylighting 12, 15
- demography 72, 73
- detectors 21, 79, 82, 83, 113
- diesel engines 17, 105
- DNA 29-35, 43, 46, 47, 66-68
- DOE-2 12, 15, 24
- dosimeters 21
- dosimetry 48, 49
- double-beta decay 83
- econometric models 25
- electric vehicles 7
- electrochemical cells 8, 86
- electrochemical energy storage 7
- electrochemistry 85, 86
- electrodes 8, 86
- electroforming 86
- electrolytes 85, 86, 89
- electron microscopy 56, 88, 105, 106
- electron storage rings 5
- electron-cyclotron resonance 6
- electronic materials 61
- electrophoresis 27, 28
- electroplating 85, 86
- endocrine system 38
- Energy Signature Monitor 12
- energy conservation 12, 13, 15
- energy consumption 25
- energy efficient buildings 12, 14, 15, 24
- energy storage 7, 8, 85
- energy-efficiency standards 24
- engines 18
- environment 19, 20, 72, 73, 114
- environmental cell 88
- environmental effects 36
- epidemiology 72, 73
- epithelial cells 33-35, 40
- erosion 63, 101, 102
- erythropoietin 29, 38
- Escherichia coli 31
- ethanol 7
- eukaryotic cells 30, 32, 42
- Euphorbias 65
- facilities 2-4, 69, 105, 109
- fatigue in steel 101
- fenestration 10, 12
- Fermilab 113
- fire models 22
- fission reactors 103
- flame radiation 19, 22
- flames 22
- flue gas 20
- flue-gas desulfurization 22
- fluorescent lamps 14
- foreign energy use 24, 25
- formaldehyde 13
- fossil fuels 36, 75, 105, 114
- free radicals 23
- free-electron laser 3, 6
- fuel cells 7, 8, 85, 86
- fuels 91, 92, 103, 105
- fusion 1, 2, 81
- fusion reactors 103
- galvanic cells 85
- gas-solid reactions 88
- gasification 9, 102, 104
- gasifiers 82
- genes 68, 69
- genetics 29-31, 42, 65, 66
- geoscience 75-77
- geothermal 75
- geothermal brines 89
- glazing 12, 15
- glazing materials 10
- grain boundaries 88
- graphite 93, 96, 102
- greenhouse effect 87
- groundwater 77
- Harderian gland 44
- heart 53, 54
- heat pump 8
- heaters 17
- heating 9
- heavy-ion beams 3, 4, 43-50, 109
- heavy-ion cancer therapy 4

- heavy-ion fusion 4
- hematopoiesis 37, 57
- high-temperature chemistry 88
- homes 12, 13, 16, 24, 25
- hormones 38
- HVAC 9
- hydrocarbons 18, 20, 65, 92, 102
- hydrodenitrogenation 103
- hydrofracture 76
- hydrogen sulfide 20
- hydrogenation 91
- ignition 18, 21
- illumination 9, 14, 15
- imaging 52-55
- indoor air 12, 13, 16, 17
- inertial confinement fusion 4
- infiltration 15
- information management 71, 72, 81
- infrared radiation 19
- insertion devices 5
- instabilities in solids 93
- instrumentation 53, 62, 75, 76, 79, 82, 83, 113
- intercalation compounds 93, 94
- internal-combustion engine 21
- ion implantation 98
- ionizing-radiation detector 1-4, 21, 43-50, 109, 110
- iridium 23
- iron, sequestering 41
- isotope separation 98
- Isotopes Project 110
- Jackson State University 59
- Josephson junction 106
- kerosene heaters 17, 18
- lasers 6, 21, 98, 104
- lead poisoning 37
- life extinction 23
- life span 43
- lighting 9, 14, 15
- linear energy transfer (LET) 43, 44, 46, 47
- lipoproteins 27, 58
- liquefaction 9, 103, 104
- liquid crystals 21
- liquid filaments 8
- low-temperature properties 95
- lungs 56
- lymphocytes 27
- magmas 75
- magnetic field effects 36
- magnetic fusion 1, 2, 81
- magnetic materials 99
- magnets 5, 99, 106
- mammalian cells 39, 45, 47
- mammary cells 33-35, 40
- marrow 27, 28, 37, 39
- materials 12, 61-63, 85-107
- materials-properties 72
- mathematics 114
- medical treatment 44-52, 55
- megakaryocytopoiesis 28, 29
- meiosis 29, 30, 42
- membrane proteins 56
- metabolism 23, 53, 55, 58
- metal chelates 20
- metal compounds 7
- metal ions 22, 67
- metallurgy 99, 100
- methylene chloride 16
- microdensitometer 54
- microparticles 10, 11
- microscopy 27, 88, 93, 105, 106
- microstructure 88, 97, 99, 100
- microtektites 23
- microwave spectroscopy 82
- minerals 75
- mirror machines 1
- mitochondria 23
- mitosis 29-31, 42
- modeling 71, 88, 91, 114
- molding 63
- molecular detector 82
- molecular interactions 89, 90, 92, 95
- molecular studies 96
- monoclonal antibodies 34
- mutagenesis 32, 39, 43, 66
- mutations 65, 66, 68
- myocardial flow 53
- National Center for Electron Microscopy 105
- national facilities 2-4, 69, 105, 109
- negative-ion sources 1, 2
- networks 71, 72
- Neutral Beam Engineering Test Facility(NBETF) 2
- neutral beams 1, 2, 81
- neutrons 46
- nitrates 18
- nitrides 63
- nitrogen fixation 23
- nitrogen heterocycles 20
- nitrous oxides 13, 20
- nonlinear dynamics 5
- Nuclear Data Sheets 111

- nuclear magnetic resonance (NMR) 106
- nuclear medicine 44-52, 55
- nuclear physics 3, 109, 110
- nuclear reactors 81, 103
- nuclear wastes 75, 77
- nucleoproteins 33
- office buildings 12, 14, 15, 24, 25
- oil 7
- oil recovery 76
- oil shale 19
- oncogenes 37, 39, 40
- oncology 47
- optical absorption 19
- optical technology 10, 12
- organic compounds 20
- organometallic chemistry 104
- organometallic species 96
- oxidants 22
- oxidation 101, 102
- ozone 38, 87
- PAREP 72
- particle accelerators 3, 4, 109, 110
- particle suspensions 10, 11
- particulates 18, 22, 56
- passive systems 9
- permanent magnets 5
- petrochemicals 92
- petroleum 75, 76
- phase stability 100
- photochemical conversion 11
- photochemistry 87, 90, 95, 98
- photoconversion 67
- photodissociation 89
- photoelectron spectroscopy 95
- photon systems 5
- photosynthesis 57, 67, 69, 89
- photothermal spectrometry 19
- photovoltaic films 19
- physics research 109, 110, 113
- plants 57, 65, 69
- plasma heating 1
- plasmas 2, 5, 6
- platelets 28, 29
- platinum 85, 89, 91, 92
- pollution 13, 16, 17, 21, 72, 91
- polymers 8, 62
- positive ion sources 1
- positron camera 52
- positron emission tomography (PET) 28, 52-55
- Positron-Electron Project (PEP) 113
- primary avian tendon (PAT) 37
- procollagen 37
- proteins 11, 32, 37, 40
- psoralens 66
- quantum electronics 98
- RAD genes 29, 30
- radiant heating 10, 11
- radiation injury 44, 45
- radiation standards 41
- radioactive beams 50, 52
- radioactive waste 75, 77
- radioactivity 69
- Radioactivity Handbook 111
- radiobiology 47
- radiographs 54
- radioimmunoassay 29
- radioisotopes 51-53, 55
- radiological physics 45
- radionuclides 41
- radiotherapy 49, 50
- radon 13, 17
- Rankine cycle cooling 10
- rapid transit 80
- reactive intermediates 104
- REC genes 31
- rechargeable cells 8, 85
- refractory materials 11, 63, 97, 99, 105
- reservoirs 75, 76
- residences 12, 13, 16, 24, 25
- respiratory diseases 56
- RNA 33, 35
- Saccharomyces cerevisiae 29, 30, 32, 42
- scale 101, 102
- scanning tunneling microscope 62
- scattering 90
- schizophrenia 54, 55
- scientists, visiting 2-4, 57, 58, 61, 69, 105, 109, 110
- scrubbers 20, 22
- SEEDIS 72, 73
- seismic technology 75, 76
- semiconductors 61, 62, 83, 98
- separation processes 9
- sequestering agents 41, 87
- shale 19
- shale oils 7
- silicon 83
- sintering 63, 97
- sky simulator 15
- sol-gel process 11
- solar cooling 9, 10
- solar energy 67-69

- solar heating 10, 11
- solid-liquid interface 89
- solid-state physics 94, 98, 100
- soot 18, 20, 22
- space 43, 46, 47, 79, 96
- spallation 102
- speciation 7
- specific heat 95
- spectroscopy 19, 21, 48, 57, 82, 83, 95, 98, 104, 106
- SQUID 106
- Stanford Linear Accelerator Center (SLAC) 113
- steels 99, 101
- stem cells 28, 37, 39
- stratosphere 87
- students 56, 61, 110
- sugar 7
- sulfates 18
- sulfur dioxide 20, 22, 91
- superconducting devices 106
- superconducting magnets 3, 99, 100, 113
- Superconducting Super Collider (SSC) 3
- superfluid states 95
- SuperHILAC 3, 4, 109
- surface coating 102
- surface erosion 63, 101, 102
- surface science 62, 85, 86
- surface treatment 105
- surfaces 19, 91, 92, 94, 95, 98
- synchrotron radiation 95
- syngas 103

- TALMS 82
- telescope 80
- tendon fibroblasts 59
- terpenes 65
- thermal energy storage 8
- thermochemical conversion 8
- thermodynamics 88, 89
- thin films 19, 86, 99

- thymus 39
- thyroid 38
- Time Projection Chamber (TPC) 113
- tokamak 1, 81
- tomography 28, 51-55
- trace constituents 21
- trace metals 18
- tracers 50, 51
- training 57, 58, 61, 110
- trains 80
- transformations interfaces 93
- transition metals 63, 92
- trees 65
- tribology 63, 101, 102
- tritium-labeling 69
- TRIUMF 113
- tumors 34, 39, 40, 42-50, 52
- turbulent combustion 19

- ultraviolet radiation 5, 43
- undulators 5
- unimolecular kinetics 20

- ventilation 12, 16
- viruses 33

- wastewater 19
- water 89, 91
- weatherization 15, 16
- welding 99, 100
- wigglers 5, 6
- window coatings 15
- windows 10, 12

- x-ray fluorescence 83
- x-ray optics 5

- yeast 29-32, 42

- zeolites 63, 103

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.