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Materials Sciences Programs
Fiscal Year 1988

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences
Washington, D.C. 20545

FOREWORD

The Division of Materials Sciences is located within the Department of Energy in the Office of Basic Energy Sciences. The Office of Basic Energy Sciences reports to the Director of the Office of Energy Research. The Director of this Office is appointed by the President with Senate consent. The Director advises the Secretary on the physical research program; monitors the Department's R&D programs; advises the Secretary on management of the laboratories under the jurisdiction of the Department, excluding those that constitute part of the nuclear weapon complex; and advises the Secretary on basic and applied research activities of the Department.

The Materials Sciences Division constitutes one portion of a wide range of research supported by the DOE Office of Basic Energy Sciences. Other programs are administered by the Office's Chemical Sciences, Energy Biosciences, Engineering and Geosciences, Advanced Energy Projects, and Carbon Dioxide Research Divisions. Materials Sciences research is supported primarily at DOE National Laboratories and Universities. The research covers a spectrum of scientific and engineering areas of interest to the Department of Energy and is conducted generally by personnel trained in the disciplines of Solid State Physics, Metallurgy, Ceramics, Chemistry, and Materials Science. The structure of the Division is given in an accompanying chart.

The Materials Sciences Division supports basic research on materials properties and phenomena important to all energy systems. The aim is to provide the necessary base of materials knowledge required to advance the nation's energy programs.

This report contains a listing of research underway in FY 1988 together with a convenient index to the Division's programs. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page.

Iran L. Thomas, Director
Division of Materials Sciences
Office of Basic Energy Sciences

RECENT DIVISION SPONSORED PUBLICATIONS

Topical and Workshop Reports[a]

- Clusters and Cluster-Assembled Materials (1988)
- Grain Boundaries and Interfaces (1988)
- Mechanisms and Physics of Crack Growth: Application to Life Prediction (1986)
- Basic Research in Ceramic and Semiconductor Science at Selected Japanese Laboratories (1987)
- Structural Ceramics: Research Status and Prospects (1986)
- Molecular Monolayers and Films (1986)[b]
- Final Report the Workshop on Conductive Polymers (1985)
- Micromechanisms of Fracture (1985)
- Polymer Research at Synchrotron Radiation Sources (1985)
- Bonding and Adhesion at Interfaces (1985)
- Corrosion-Resistant Scales in Advanced Coal Combustion Systems (1985)
- Novel Methods for Materials Synthesis (1984)[c]
- Theory and Computer Simulation of Materials Structures and Imperfections (1984)
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Coatings and Surface Modifications (1983)[c]
- High Pressure Science and Technology (1982)
- Scientific Needs of the Technology of Nuclear Waste Containment (1982)
- Radiation Effects (1981)
- Condensed Matter Theory and the Role of Computation (1981)
- Research Opportunities in New Energy-Related Materials (1981)[c]
- Aqueous Corrosion Problems in Energy Systems (1981)[c]
- High Temperature Corrosion in Energy Systems (1981)[c]
- Basic Research Needs and Opportunities on Interfaces in Solar Materials (1981)[c]
- Basic Research Needs on High Temperature Ceramics for Energy Applications (1980)[c]

Description of Research Facilities, Plans, and Associated Programs

- Centers for Collaborative Research[a]
- Materials Sciences Division - Long Range Plan (1984)[a]
- Office of Basic Energy Sciences 1986 Summary Report (1986)

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[a] Available in limited quantities from the Division of Materials Sciences.

[b] Also published in Langmuir.

[c] Also published in Materials Science and Engineering.

OFFICE OF BASIC ENERGY SCIENCES
Division of Materials Sciences Structure

Division of Materials Sciences

Director: I. L. Thomas

(Taree R. Thompson - Secretary)
(301) 353-3427

Metallurgy and Ceramics Branch

Chief: I. L. Thomas (Acting)

(Judy McFarland - Secretary)
(301) 353-3428

R. J. Gottschall
J. B. Darby
J. L. Routbort 1/
R. W. Heckel 2/

Solid State Physics and Materials Chemistry Branch

Chief: B. C. Frazer

(Christie Goodrich - Secretary)
(301) 353-3426

R. D. Kelley
J. J. Smith
W. A. Kamitakahara 3/
C. C. Herrick 4/

Notes: 1/ On detail from Argonne National Laboratory
2/ On assignment from Michigan Technological University
3/ On detail from Ames Laboratory
4/ On detail from Los Alamos National Laboratory

INTRODUCTION

The purpose of this report is to provide a convenient compilation and index of the DOE Materials Sciences Division programs. This compilation is primarily intended for use by administrators, managers, and scientists to help coordinate research.

The report is divided into seven sections. Section A contains all Laboratory projects, Section B has all contract research projects, Section C has projects funded under the Small Business Innovation Research Program, Sections D and E have information on DOE collaborative research centers, Section F gives distribution of funding, and Section G has various indexes.

The FY 1988 funding level, title, personnel, budget activity number (e.g., 01-2) and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), Materials Chemistry (03), or Facility Operations (04). The budget numbers carry the following titles:

01-1 - Structure of Materials
01-2 - Mechanical Properties
01-3 - Physical Properties
01-4 - Radiation Effects
01-5 - Engineering Materials

02-1 - Neutron Scattering
02-2 - Experimental Research
02-3 - Theoretical Research
02-4 - Particle-Solid Interactions
02-5 - Engineering Physics

03-1 - Synthesis & Chemical Structure
03-2 - Polymer & Engineering Chemistry
03-3 - High Temperature & Surface Chemistry

04-1 - Facility Operation

Sections D and E contain information on special DOE centers that are operated for collaborative research with outside participation. Section F summarizes the total funding level. In Section G the references are to the project numbers appearing in Sections A, B, and C and are grouped by (1) investigators, (2) materials, (3) techniques, (4) phenomena, and (5) environment.

It is impossible to include in this report all the technical data available for the program in the succinct form of this Summary. To obtain more detailed information about a given research project, please contact directly the investigators listed.

Preparation of this FY 1988 summary report was coordinated by I. L. Thomas. Though the effort required time by every member of the Division, much of the work was done by T. Thompson, J. McFarland, and C. Goodrich.

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SECTION A

Laboratories

The information in this section was provided by the Laboratories. Most projects are of a continuing nature. However, some projects were concluded and others initiated this fiscal year.

AMES LABORATORY
Iowa State University
Ames, IA 50011

D. K. Finnemore - Phone (515) 294-4037

Metallurgy and Ceramics - 01 -

R. B. Thompson - Phone (515) 294-4446

001. MATERIALS SCIENCE OF INTERFACES

A. J. Bevolo
Phone: (515) 294-5414

$134,000 01-1

Studies of interface structure and composition using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Auger and reflection electron loss spectroscopy of metallic hydrides for phase identification and mapping. Scanning Auger microprobe analysis of effects of radiation on the competition between C and P grain boundary segregation in iron. Local chemical state information from Auger lineshape analysis in metallic glasses. Electronic structure of heavy fermion metals and binary transition metal alloys. Surface segregation in binary solid-solution alloys.

002. SOLIDIFICATION MICROSTRUCTURES

R. K. Trivedi, J. D. Verhoeven, R. W. McCallum, L. S. Chumbley
Phone: (515) 294-5869

$270,000 01-1

Studies of solidification processes and their applications to technologically important materials. Theoretical and experimental studies of the effect of temperature gradient, growth rate and composition on the stability and steady-state shape of solid-liquid interfaces obtained during controlled solidification. Study of morphological transition from dendritic to cellular to eutectic structure. Study of interface stability and morphological characteristics in model transparent material such as succinonitrile and acetone mixture. Directional solidification studies on [redacted] and morphology in gray, nodular, and white cast iron. Solidification processing of $(Dy,Tb)Fe_2$ magnetostrictive alloys, Nd-Fe-B permanent magnet materials, and intermetallic compounds, and analysis of their magnetic and mechanical properties.

AMES LABORATORY (continued)

003. CONTROL AND ANALYSIS OF MICROSTRUCTURES

J. D. Verhoeven, L. S. Chumbley, R. W. McCallum, A. J. Bevolo,
Phone: (515) 294-9471

$602,000 01-1

Studies of processing procedures and analysis of resulting microstructures and properties. Evaluation of microstructural changes in the austempering of nodular cast irons. Study of surface characteristics of in situ Cu-refractory metal alloys. Study of magnetic properties of in situ Cu-Fe-Co alloys. Characterization of the microstructure and study of the resulting electronic transport and magnetic properties of high T_c superconducting materials.

004. MECHANICAL METALLURGY

W. A. Spitzig, J. Kameda, B. Biner
Phone: (515) 294-5082

$500,000 01-2

Studies of the effects of environment and stress on the mechanical properties of metals. Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Interstitial effects on strength and ductility in both nonhydrogenated and hydrogenated V, Nb, and Ta. Investigation of hydrogen diffusion in vanadium-base alloys by internal friction. Hydrogen-induced brittle cracking in both low and high hydrogen solubility bcc metals and alloys. Effects of radiation-induced defects and solute segregation on [redacted] embrittlement. Modeling of hydrogen embrittlement. Description of three dimensional arrays of defects and relationship of arrangement to ductility and mechanical properties. Correlation between defect structure and nondestructive measurement. Evaluation of origin of strengthening in heavily deformed metal-metal composites. Use of this information in defining new processing procedures.

005. RARE EARTH MATERIALS

K. A. Gschneidner Jr.
Phone: (515) 294-2272

$370,000 01-3

Quenching of spin fluctuations and other magnetic phenomena in: (1) highly enhanced paramagnets RCo_2 (R=Sc, Y and Lu), Sc and Pd-Ni alloys, (2) valence fluctuation materials $CeSn_x$ and $CeSi_x$ alloys, and (3) itinerant ferromagnets Sc_3In and $ZrZn_2$. Low-temperature, high-field heat capacity, magnetic susceptibility, electrical resistance and lattice parameters are used to characterize the behaviors. Nonequilibrium phases resulting from solidification and phase transformations in rare-earth-based alloys.

AMES LABORATORY (continued)

006. NDE MEASUREMENT TECHNIQUES

O. Buck, R. B. Thompson, B. Biner
Phone: (515) 294-3930

$547,000 01-5

Techniques to measure failure-related material properties to improve understanding of failure mechanisms and inspection reliability. Ultrasonic measurement of internal stresses, texture, and porosity. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide information about closure near crack tip and its influence on crack growth rate and detectability. Acoustic microscopy techniques for high resolution studies of elastic and anelastic structure. Relationship between fatigue damage, stress and microstsructure to magnetic properties.

007. ADVANCED MATERIALS AND PROCESSES

F. A. Schmidt, I. E. Anderson
Phone: (515) 294-5236

$348,006 01-5

Development of advanced processes for preparing special metals. Development of new melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys. New thermite reduction process for preparing rare earth-iron alloys and for producing oriented crystallites of magnetostrictive compounds. Processing of stoichiometric and non-stoichiometric materials by an inducively coupled plasma. Electrotransport and zone melting for maximum purification of rare earth and refractory metals. Processing of single crystals of congruent melting and peritectic materials by levitation zone melting, free-standing vertical zone melting, Bridgman, Czochralski and strain-anneal recrystallization. Total consumption flame processing and high pressure gas atomization for production of fine powders of metals and mixed metal oxides. Above research being conducted in the Materials Preparation Center described in the Section-Collaborative Research Centers.

AMES LABORATORY (continued)

008. HIGH TEMPERATURE SUPERCONDUCTING WIRE

R. W. McCallum, J. D. Verhoeven, I. E. Anderson
Phone: (515) 294-4736

$595,000 01-5

Investigation of techniques for fabrication of bulk wire from high T_c, copper-oxide based superconductors. Wire fabrication by mechanical reduction of powdered oxides encapsulated iin Ag cylinders. Studies of the effects of powder quality and O_2 treatment on superconducting properties. Determination of phase diagrams. [redacted], including local structure and grain boundary cracking. Development of improved techniques for producing fine grained and/or grain aligned bulk materials.

009. SCIENTIFIC AND TECHNOLOGICAL INFORMATION EXCHANGE

F. A. Schmidt, E. O. Feinberg, T. E. Wessels
Phone: (515) 294-5236

$135,000 01-5

Dissemination of information to the scientific and industrial communities. Publication of High-T_c Update for rapid dissemination of up-to-date information on high-temperature superconductivity research. Operation of Materials Referral System and Hotline to accumulate information from all known National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community.

Solid State Physics - 02 -

B. N. Harmon - Phone: (515) 294-7712

010. NEUTRON SCATTERING

W. A. Kamitakahara, C. Stassis, J. Zarestky
Phone: (515) 294-4224

$440,000 02-1

Magnetic properties of high temperature superconductors (La_2CuO_4 ...). Study of the lattice dynamics, thermodynamic properties, and structural transformations of metals at high temperatures (bcc and fcc La), structure and diffusion in metal hydrides (ScH_x, LaH_x), dynamics and phase transitions of alkali-graphite intercalation compounds, electronic structure and phonon spectra of mixed valence compounds ($CePd_3$, α-Ce, $YbAl_{12}$), relation of electron-phonon interaction to superconductivity (La, $LaSn_3$). High pressure studies (α-Ce, La). Study of the magnetic properties of heavy fermion superconductors ($CeCu_2Si_2$, UPt_3, UBe_{13}).

AMES LABORATORY (continued)

011. SEMICONDUCTOR PHYSICS

H. R. Shanks, J. Shinar
Phone: (515) 294-6816

$235,000 02-2

Preparation and characterization of thin films, rf sputter desposition of amorphous semiconductors including aSi, aSi-C, aGe, aGe-C and crystalline AlN. Heteroepitaxy on compound substrates, and quantum well structures. Surface and interface characterization with LEED, Auger, LEELS, photodeflection and IR absorption spectroscopy. Measurements of gap state densities using DLTS, SCLC, ODMR, and C-V on Schottky barriers.

012. SUPERCONDUCTIVITY

D. K. Finnemore, J. E. Ostenson
Phone: (515) 294-3455

$400,000 02-2

Preparation, characterization, and study of the fundamental properties of copper oxide superconductors; search for new superconducting materials; current transfer and the proximity effect near superconductor normal metal interfaces, interaction between superconducting and magnetic properties, studies of single quantized vortices for use in microprocessors and logic devices; development of superconducting composites for large scale magnets.

Fundamental studies of superconductivity in metal-metal composites, use of Josephson junctions to study flux pinning of isolated vortices, development of materials with very low pinning, development of superconducting composites suitable for large scale magnets in the 8 to 16 Tesla range, practical studies to improve wire fabrication techniques, development of magnetic shielding devices, study of magnetostrictive materials.

013. OPTICAL, SPECTROSCOPIC, AND SURFACE PROPERTIES OF SOLIDS

D. W. Lynch, C. G. Olson, M. Tringides
Phone: (515) 294-3476

$535,000 02-2

Electron photoemission and optical properties (transmission, reflection, ellipsometry) of solids in the visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation; low energy electron diffraction, scanning tunnelling microscopy. Ce and Ce- compounds (e.g., $CeSn_3$) heavy Fermion systems, e.g., UPt_3, Fe-based alloys with Si, FeRh, copper-oxide-based superconductors, photon- and electron-stimulated desorption of neutral atoms from insulators; O on W. Fundamental studies of surface roughening and annealing, island growth, etc. using LEED line shape analysis.

AMES LABORATORY (continued)

014. NEW MATERIALS AND PHASES

D. C. Johnston, R. G. Barnes, C. A. Swenson, D. R. Torgeson
Phone: (515) 294-5435

$570,000 02-2

Synthesis and characterization of new high T_c superconductors as well as ternary compounds such as Chevrel phases, ternary transition metal borides and rare-earth transition metal silicides and phosphides. Study of the physical properties of these new materials, such as microhardness, phase equilibria, their refractory nature, and high temperature behavior. Properties of new ternary phases at low temperatures, including magnetic susceptibility, transport properties, heat capacity, crystallographic phase transformations, coexistence of superconductivity and long range magnetic order. High pressure equations of state of new materials, elementary solids (ternary compounds and alloys, and alkaline earth metals), low temperature expansivity and heat capacity of materials (Lu) containing hydrogen. Applications of NMR to hydrogen embrittlement of refractory metals (V, Nb, Ta) and alloys (V-Ti, Nb-V), trapping of hydrogen by interstitial impurities in these metals, structural and electronic characterization of hydrogenated amorphous Si, Ge, SiC, and GeC films.

015. X-RAY DIFFRACTION PHYSICS

A. I. Goldman
Phone: (515) 294-3585 or 294-9614

$200,000 02-2

X-ray measurements on Icosahedral Phase alloys, high T_c ceramic superconductors, magnetic structures and phase transitions, and solids at high pressure. Participation in the MATRIX PRT beam line at NSLS.

016. ELECTRONIC AND MAGNETIC PROPERTIES

B. N. Harmon, K.-M. Ho, M. Luban, C. T. Chan, C. Soukoulis
Phone: (515) 294-7712

$480,000 02-3

Magnetic properties of new high T_c superconductors. Theoretical studies of bulk and lattice dynamical properties of materials using first principles total energy calculation. Anharmonic interaction, lattice instabilities, phase transformation, electron-phonon interaction, and superconductivity. Equations of state (pressure and temperature). Hydrogen-metal interactions. Electron localization in disordered materials. Magnetism in spin glasses and ternary compounds. Electronic structure of rare earth compounds and transition metal sulfides and hydrides. Theory of amorphous semiconductors, and nuclear magnetic ordering in metals.

AMES LABORATORY (continued)

017. OPTICAL AND SURFACE PHYSICS THEORY

R. Fuchs, K.-M. Ho
Phone: (515) 294-3675

$125,000 02-3

Optical properties of metals, semiconductors, and insulators, studies of surfaces, thin films, layered systems, small particles, and powders. Differential surface reflectance spectroscopy. Raman scattering from molecules adsorbed on metal surfaces. Surface electronic structure of metal electrodes (e.g., Ag), electroreflectance, and microscopic properties of the metal-electrolyte interface. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrosion effects, anodic photocurrents, the liquid-metal interface. First principles calculation of lattice relaxation, reconstruction and phonons at single crystal surfaces (Al, Au, W, Mo).

018. SUPERCONDUCTIVITY THEORY

J. R. Clem, V. G. Kogan
Phone: (515) 294-4223

$160,000 02-3

Electrodynamic behavior of current-carrying CuO-based high T_c superconductors containing magnetic flux. Flux-line cutting and flux pinning in arrays of nonparallel vortices. Superconducting magnetic shielding. Critical fields and critical currents of proximity-coupled superconducting-normal (SN) multilayers and composites. Properties of Josephson and SNS junction arrays. 1/f noise and sensitivity to trapped magnetic flux in SQUIDs.

AMES LABORATORY (continued)

Materials Chemistry - 03 -

T. J. Barton - Phone: (515) 294-7712

019. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS

J. D. Corbett, R. E. McCarley, R. A. Jacobson
Phone: (515) 294-3086

$441,000 03-1

Synthesis, structure and bonding in intermetallic systems-new Zintl phases, new ternary compounds stabilized by interstitials. Reactions and stabilities of phases in the system $CsI-Zr-ZrI_4-ZrO_2$, effects of common impurities, the fate of the important fission products. Synthesis, structure and properties of new ternary oxide phases containing heavy transition elements, especially metal-metal bonded structures stable at high temperatures. Low temperature routes to new metal oxide, sulfide and nitride compounds. Correlation of structure and bonding with d-electron count and physical properties. Development of diffraction techniques for single crystal and non-single crystal specimens, techniques for pulsed-neutron and synchrotron radiation facilities, and use of Patterson superposition methods. Experimental methods include X-ray diffraction, photoelectron spectroscopy, resistivity and magnetic susceptibility measurements, high temperature reactions and synthesis of molecular precursors.

020. CERAMIC MATERIALS

T. J. Barton, L. E. Burkhart, G. Burnet, M. J. Murtha
Phone: (515) 294-7655

$457,000 03-2

Synthesis of silicon-nitrogen polymers. Study of controlled thermal decomposition of preceramic polymers. Development of thermal and photochemical routes to transient compounds containing silicon-nitrogen multiple bonds as route to preceramic materials. Kinetics and mechanisms of thermal decomposition of variously substituted silylamines. Techniques include plasma-induced polymerization, flash vacuum pyrolysis, solution photochemistry, condensation polymerization. Synthesis and characterization of materials (metal oxides and sulfides, silicon nitride precursors) for ceramic powders and thin films, with emphasis on liquid-phase methods such as homogeneous precipitation and microemulsion techniques, preparation and use of monodisperse powders in ceramics and catalysis. Studies of nucleation, growth, and agglomeration phenomena for control of precipitation and film deposition. Theoretical studies include DLVO theory for particle-particle interactions, coagulation and population balance equations for agglomeration kinetics. Investigation of reaction mechanisms and kinetics for high temperature reactions in the carbochlorination and carbonitrification processes to produce non-oxide ceramics.

AMES LABORATORY (continued)

021. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS

H. F. Franzen, J. W. Anderegg
Phone: (515) 294-5773

$238,000 03-3

Study of refractory and corrosion-resistant materials such as transition metal aluminides (Zr-Al, Ta-Al), phosphides and sulfides by both experimental and theoretical techniques to understand the relationships among crystal structure, chemical bonding, and electronic structure as they affect high temperature stability, phase equilibria, and order-disorder transitions. Experimental methods include X-ray and electron diffraction for structure analysis, computer automated simultaneous mass loss-mass spectrometry for high temperature vaporization reactions related to stability, and photoelectron spectroscopy for the electronic structure of solids. Electronic structure studies also include a program of band structure calculations. High temperature X-ray powder diffraction is routinely used.

022. SURFACE CHEMISTRY

R. S. Hansen, K. G. Baikerikar, D. C. Johnson, P. A. Thiel
Phone: (515) 294-2770

$506,000 03-3

Evaluation of mechanisms of catalytic reactions, especially hydrogenation, hydrogenolysis, methanation, and hydrodesulfurization reactions, by surface characterization and kinetic techniques, with emphasis on single crystal and evaporated film catalysts. Study of lubrication phenomena: decomposition pathways and products of fluorinated organic molecules at surfaces. Mechanisms of corrosive oxidation of metals. Chemistry of electrode reactions, including electrocatalysis and corrosion reactions. Characterization of electrocatalytic materials by modulated hydrodynamic voltammetry. Reactivity of oxidized and doped electrode surfaces, including characterization of oxygen mobility and defect density at such electrodes. Surface chemistry of nucleation and flocculation applied to ceramic processing. Techniques used include low energy electron diffraction, Auger and scanning Auger electron spectroscopy, infra-red emission and electron energy loss spectroscopies, ring-disk and modulated hydrodynamic voltammetry.

ARGONNE NATIONAL LABORATORY
9700 S. Cass Avenue
Argonne, IL 60439

F. Y. Fradin - Phone (FTS) 972-3504 or (312) 972-3504

Metallurgy and Cermamics - 01 -

B. Dunlap - Phone (FTS) 972-4925 or (312) 972-4925
H. Wiedersich - Phone (FTS) 972-5079 or (312) 972-5079

040. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

N. J. Zaluzec, C. W. Allen, C. R. Bradley
Phone: (312) 972-5075

$1,590,000 01-1

Development and use of high-voltage and high-spatial resolution analytical microscopy for materials research. Operation and development of the Center's 1.2 MeV High-Voltage Electron Microscope-Tandem Facility with in situ capability for direct observation of ion-solid interactions. The HVEM is currently being utilized for research programs in advanced materials, mechanical properties, irradiation effects, oxidation and hyd rogenation effects. HVEM specimen stages are available for heating (1300 K), cooling (10 K), straining, resistivity and gaseous environments. Ion-beam interface with 100 kV ion accelerator and 2 MV tandem accelerator available for in situ implantations and irr adiations. A 650 kV ion accelerator is being procured as a replacement for the 300 kV instrument. Approximatey 50 percent of HVEM 50 percent of HVEM usage is by non-ANL scientists on research proposals approved by the Steering Committee for the Center that meets every 6 months. A state-of-the-art, medium-voltage, ultra-high vacuum, field-emission gun, Analytical Electron Microscope is being procured. Its design is directed toward the attainment of the highest mic roanalytical resolution and sensitivity. Fundamental studies of electron-solid interactions and microcha rac terization of materials, using TEM, STEM, XEDS, and EELS are conducted at present on conventional transmission electron microscopes (JEOL 100CX, Philips EM420, and Philips CM30).

ARGONNE NATIONAL LABORATORY (continued)

041. BASIC CERAMICS

D. J. Lam, S. K. Chan, M. V. Nevitt, J. L. Routbort, S. J. Rothman, B. W. Veal
Phone: (312) 972-4966

$1,394,000 01-3

Experimental and theoretical studies of electronic and atomic structure, phase stability, phase transformation kinetics, electronic and ionic transport, and mechanical properties in multicomponent (including high T_c superconducting) oxides. X-ray photelectron (XPS) and X-ray absorption (XANES and EXAFS) spectrosopic studies of structural and electronic properties. Thermal and lattice property studies using heat capacity, EXAFS, Billouin scattering, and ultrasonic measurements. Crystal chemistry and structural phase transformation studies of high T_c superconducting oxides using X-ray and neutron diffraction, electrical conductivity, and Meissner effect measurements. Diffusion mechanisms and point defect studies in oxides as a function of oxygen partial pressure at high temperature using cation and oxygen tracer diffusion, and electrical conductivity measurements. Development of the embedded molecular cluster code to calculate electronic structure, cohesive energy, and defect interaction energy of complex oxides. Development of non-classical theory of nucleation for martensitic transformations in oxide systems. Preparation of single crystals of high T_c superconducting oxides and monoclinic phase of ZrO_2 with and without dopants.

042. [redacted]

K. L. Merkle, J. N. Mundy, and D. N. Seidman
Phone: (312) 972-4990

$714,000 01-3

Experimetal studies of solid interfaces. Atomic structure of grain boundaries in oxides and metals. Nature and properties of large-angle grain boundaries, role of boundary plane, and comparisons to computer models. [redacted] and segregation to grain boundaries. Structure and composition of phase boundaries on an atomic scale with special focus on metal-ceramic interfaces. Experimental techniques include high-resolution electron microscopy, analytical electron microscopy, secondary ion mass spectroscopy, radiotracer techniques, atom-probe field-ion microscopy as well as ion- and X-ray scattering techniques.

ARGONNE NATIONAL LABORATORY (continued)

043. IRRADIATION AND KINETIC EFFECTS

L. E. Rehn, R. C. Birtcher, M. A. Kirk, N. Q. Lam, P. R. Okamoto, U. Scheuer, R. P. Sharma, F-R. Ding, A. Liu, S. Tang
Phone: (312) 972-5021

$1,254,000 01-4

Investigations of mechanisms leading to the formation of defect aggregates, precipitates, and other inhomogeneous distributions of atoms in solids with and without displacement-producing irradiation. Surface layer modification of alloys by ion implantation, ion-beam mixing, and sputtering. Radiation-induced segregation to internal and external defect sinks. Radiation-enhanced diffusion. Effects of irradiation on alloy composition, microstructure, superconductivity, and amorphization. Displacement cascades. Inert-gases in solids. Effects of amorphizations on dimensional stability. In situ studies of ion and electron bombardment in the High-Voltage Electron Microscope. Neutron and dual-beam ion irradiation. Computer modeling of irradiation-induced microstructural changs. Ion-beam analysis. Radiation sources include HVEM-2MV Tandem facility and two 300-kV ion accelerators.

044. AMORPHOUS AND NANOPHASE MATERIALS

L. E. Rehn, P. R. Okamoto, J. Eastman, R. Siegel, W. J. Meng, A. Narayamasamy, F. R. Ding, Y. Liao
Phone: (312) 972-5021

$720,000 01-5

Investigations of the synthesis of amorphous and nanophase materials by inert-gas condensation and subsequent compaction. Amorphization by isothermal solid-state reactions at the interfaces of vapor-deposited multilayer films and mixed metal powders, by ion-beam mixing of multilayer films, and by displacement damage of intermetallic compounds by electron and ion beams. Elastic properties measurements in ordered, disordered and amorphous alloys. In situ high-voltage electron microscopy studies of the morphology and kinetics of the crystalline-to-amorphous transformations. Mechanical properties and sintering characteristics of nanophase ceramics. Synthesis of ultra-fine metallic powders. Materials characterization methods include X-ray and neutron diffraction, electron microscopy, electrical resistivity, Rutherford backscattering, AES, EELS, and EXAFS.

1,974,000

ARGONNE NATIONAL LABORATORY (continued)

045. HIGH T_c SUPERCONDUCTOR DEVELOPMENT

B. D. Dunlap, K. Goretta, R. B. Poeppel, J. Routbort, D. Shi
Phone: (312)-972-5538
$500,000 01-5

Development of a short length, current-carrying, ceramic superconductor made by tape-casting, extrusion, powder-in-tubes, thick-film techniques, co-evaportion, plasma and flame spraying, and/or reactive sputtering. Studies of scaling-up of powder preparation. Mechanisms and improvements of flux pinning and J_c enhancement in applied fields will be studied and used to reach stated goal of 10,000 A/CM^2 at 77K and 2T applied fields. Collaborative research with scientists at Ames Laboratory and Brookhaven National Laboratory.

Solid State Physics - 02 -

B. Dunlap - Phone (FTS) 972-4925 or (312) 972-4925
M. B. Brodsky - Phone (FTS) 972-5016 or (312) 972-5016

046. NEUTRON AND X-RAY SCATTERING

J. D. Jorgensen, T. O. Brun, J. E. Epperson, J. Faber, G. P. Felcher, R. Kleb, D. L. Price, S. Susman, R. Dejus, S-Y. Pei
Phone: (312) 972-5513
$1,825,000 02-1

Exploitation of neutron and X-ray scattering techniques in the study of the properties of condensed matter. Instrument development and interactions with university and industrial users at IPNS. Investigations of the structure and defects of intermetallic and oxide superconductors, structure and dynamics of chalcogenide and oxide glasses, surface magnetism, alloy decomposition and mixing, defects in nonstoichiometric oxides, spectroscopy of hydrocarbons and template molecules in zeolite catalysts, atomic momentum distributions with deep inelastic scattering, and fast ion transport in solids.

ARGONNE NATIONAL LABORATORY (continued)

047. SUPERCONDUCTIVITY AND MAGNETISM

B. D. Dunlap, G. W. Crabtree, K. E. Gray, D. G. Hinks, A. J. Fedro, B. Dabrowski, W. Kwok, D. R. Richards
Phone: (312) 972-5538

$1,527,000 02-2

Experimental and theoretical investigations of the magnetic and superconducting properties of materials. Strong emphasis is being placed on studies of high-T_c oxide superconductors. Other programs include studies of the electronic properties of mixed valence, heavy fermion and other narrow-band materials containing rare-earth and actinide elements. Experimental techniques include the de Haas-van Alphen effect, Mossbauer spectroscopy, transport and magnetic measurements, electron tunneling, heat capacity, positron annihilation, materials preparation and characterization.

048. TWO-DIMENSIONAL MATERIALS

S. D. Bader, M. B. Brodsky, M. Grimsditch, C. Liu, E. R. Moog, W. Robertson, and K. Yang
Phone: (312)-972-4960

$963,000 02-2

Research on the growth and physical properties of novel ultra-thin, epitaxial films, metallic sandwiches, superlattices and superconductors. Thin-film and surface-science preparation techniques include molecular beam epitaxy, evaporation and sputtering. Monolayer growth phenomena and interfacial structure characterization methods include electron (RHEED and LEED) and X-ray diffraction. Electronic properties studied via electron spectroscopies (AES, UPS, XPS, STM), band-structure theory, and low-temperature transport, magnetic and high-T_c superconductivity measurements. Elastic, magnetic and vibrational properties using Brillouin and Raman scattering. Magnetic studies using the magneto-optic Kerr effect and spin-polarized photoemission.

049. PHOTON SCIENCE AT SYNCHROTRONS

G. K. Shenoy, E. E. Alp, S. D. Bader, J. M. Bloch, J. C. Campuzano
Phone: (312) 972-5537

$500,000 02-2

Experimental investigations using various synchrotron radiation sources of electronic properties of materials. Understanding of the narrow-band phenomenon. Measurements of the structure of surfaces and interfaces using surface scattering techniques. Study of actinides and high T_c oxide superconductors using X-ray absorption spectroscopy.

ARGONNE NATIONAL LABORATORY (continued)

050. CERAMIC EPITAXY AND MULTILAYER STRUCTURE

D. J. Lam, H. L. Chang
Phone: (312) 972-4966

$250,000 02-2

Coordinated experimental and theoretical research program on the processing, characterization, and property determination of epitaxial ceramic films and layered composites prepared by organometallic chemical vapor deposition techniques. A variety of experimetal and theoretical techniques are used to study this problem; these include electrical conductivity and optical property measurements, conventional and high-resolution transmission electron microscopy, photoelectron spectroscopy, secondary ion mass spectroscopy, X-ray diffraction, ab initio quantum mechanical calculations and computer simulations.

051. CONDENSED MATTER THEORY

D. D. Koelling, R. Benedek, R.K. Kalia, M. Norman, K. Strandburg, P. Vashishta
Phone: (312) 972-5507

$1,115,000 02-3

Condensed matter theory in statistical physics, electronic band structure, and many body effects. Molecular-dynamics modeling of microclusters and glasses. Spatial and electronic structure of covalent glasses. Transport and structural transformations in ionic conductors. Fragmentation of clusters. Models for quasicrystal structure. Electronic structure calculations of narrow-band metal and alloy systems. Positron annihilation characteristics in metals and alloys. Phenomenological incorporation of fluctuation phenomenon generating mass enhancement and mechanism of superconductivity in heavy fermion materials. Studies of the new copper oxide based superconductors. Systems incorporating both atomic motion and electronic structure utilizing new optimization techniques.

ARGONNE NATIONAL LABORATORY (continued)

052. MODELING AND THEORY OF INTERFACES

D. Wolf, J. Lutsko, S. Phillpot, A. J. Freeman, S. Yip
Phone: (312) 972-5205

$240,000 02-3

Computer simulation of the physical properties of grain and interphase boundaries between dissimilar materials, involving both atomistic simulation methods (lattice statics and dynamics, molecular dynamics, Monte-Carlo) and electronic structure calculations. The latter are aimed at calculating certain relatively simple bulk and defect properties directly (i.e., without assumption of potentials) which can then be compared with atomistic-simulation results of the same property. The atomistic simulations are used to determine, for example, the structure and free energy of solid interfaces as a function of temperature, the point-defect properties of interfaces such as impurity segregation and diffusion, and the properties of voids in grain boundaries and in the bulk. Materials considered involve metals, semiconductors and ceramics as well as interfaces between them.

[redacted] ULTRA-HIGH FIELD SUPERCONDUCTORS

K. E. Gray, R. T. Kampwirth, J. Kang
Phone: (312) 972-5525

$384,000 02-5

Emphasis is for the development of a low-temperature, high-rate sputtering process for the new high-temperature, high-field oxide superconductors. Films of the $YBa_2Cu_3O_7$, Bi-Sr-Ca-Cu-O and Tl-Ba-Ca-Cu-O systems have been successfully made using conventional high-temperature annealing. The effort includes the effects of preparation conditions, substrate type, annealing steps and target composition on the superconducting properties. Material characterization by X-ray, SEM, TEM, RBS, ICPAES. Layered NbN/AlN films exhibiting 4-5 times higher critical current density will also be addressed.

ARGONNE NATIONAL LABORATORY (continued)

Materials Chemistry - 03 -

B. Dunlap - Phone (FTS) 972-4925 or (312) 972-4925
D. M. Gruen - Phone (FTS) 972-3513 or (312) 972-3513

054. CHEMICAL AND ELECTRONIC STRUCTURE

J. M. Williams, M. A. Beno, C. D. Carlson, A. J. Schultz, H. H. Wang, U. Geiser, L. C. Porter
Phone: (312) 972-3464

$1,115,000 03-1

New materials synthesis and characterization focusing on synthetic organic metals and superconductors based on BEDT-TTF (bis-ethylenedithiotetrathio-fulvalene) and various new organic donor molecules. Development of structure-property relationships. Electrical properties measurements. Development of improved crystal growth techniques. Continuing development of the neutron time-of-flight single-crystal diffractometer (SCD) at the Intense Pulsed Neutron Source (IPNS). Phase transition and crystal structure studies as a function of temperature (10-300 K) using the IPNS-SCD and a low-temperature (10 K) X-ray instrument.

055. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

M. Blander, L. A. Curtiss, M-L. Saboungi
Phone: (312) 972-4548

$509,000 03-2

Experimental and theoretical investigations of important thermodynamic and structural properties of ordered and associated solutions and amorphous (metastable) materials. Thermodynamic and structural measurements (e.g., emf, vapor pressure, neutron diffraction) are combined with theoretical calculations (e.g., molecular dynamics, statistical mechanics) to determine the fundamental characteristics of ordered and associated solutions (e.g., chloroaluminates, ionic alloys, silicates). Other techniques such as small angle neutron scattering, and inelastic neutron scattering are used to obtain data relating to valence states, ordering and clustering of atoms and ions in solution. The extension of theories and concepts for pyrometallurgy is explored.

ARGONNE NATIONAL LABORATORY (continued)

056. INTERFACIAL MATERIALS CHEMISTRY

D. M. Gruen, V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, M. Blander
Phone: (312) 972-3513

$496,000 03-2

Complementary fundamental research activities that focus on the structural, electronic, and catalytic properties of macro-molecular and cluster-type systems such as zeolites and transition metal clusters. Studies of new transition metal-containing zeolites by extended X-ray absorption fine structure, electron paramagnetic resonance, nuclear magnetic resonance, Mossbauer, and infrared spectroscopies, as well as by high-voltage electron microscopy, neutron inelastic scattering spectroscopy and ab initio molecular orbital theory, with the aim of elucidating the relationship between zeolite structure and catalytic activity/selectivity. Ab initio molecular orbital calculations, alone or in combination with statistical mechanical analyses, on polynuclear metal clusters and on molecule/surface interactions in zeolite-like environments that yield incisive knowledge of adsorbate-substrate interactions on a molecular level. Molecular orbital calculations on clusters modeling high T_c superconductors. Synethesis of high T_c materials using alloy precursors.

057. AQUEOUS CORROSION

D. M. Gruen, V. A. Maroni, L. A. Curtiss, J. Frye, C. A. Melendres, Z. Nagy, M. J. Pellin, R. M. Yonco, N. C. Hung
Phone: (312) 972-3513

$639,000 03-2

Basic research aimed at elucidating fundamental aspects of aqueous corrosion under conditions of temperature and pressure (300^{o}C and 10 MPa) relevant to light water fission reactor environments. Investigations of the mechanisms responsible for passivation on iron and nickel-based alloys and for crack and pit propagation in these same alloys. Studies of the details that connect surface adsorption, electron transfer, and electrolyte chemistry with passive film structure using a combination of in situ surface sensitive spectroscopic methods and transient electrochemical techniques. In situ measurements of metal/solution interfaces using laser Raman, Ramn-gain, and second harmonic generation spectroscopies. Investigations of the key features of the interfacial chemistry associated with passivation processes (including charge transfer kinetics) using pulsed galvanostatic/ potentiostatic, dc polarization, and ac impedance through the application of molecular dynamics methods in combination with ab initio molecular orbital theory.

ARGONNE NATIONAL LABORATORY (continued)

058. PARTICLE AND PHOTON INTERACTIONS WITH SURFACES

D. M. Gruen, W. F. Calaway, J. Chen, A. R. Krauss,
G. J. Lamich, M. J. Pellin, C. E. Young
Phone: (312) 972-3513

$1,030,000 03-3

Development of multiphoton resonance ionization methods combined with energy and angle refocusing time-of-flight mass spectroscopy for ultrasensitive detection of sputtered species. Application of this technique to studies of (1) fundamental problems in surface science (depth of origin of sputtered species; sputtering of metal clusters; adsorbate structures; strong metal support interactions; mechanisms of oxidation; surface segregation), (2) electron- and photon-induced desorption cross sections and mechanisms for neutral species with particular reference to desorption by synchrotron radiation, (3) trace analysis for selected systems of special significance such as impurities in semiconductors, (4) fundamental damage mechanisms in optical materials exposed to high power laser fluxes.

Surface composition, structure and radiation-enhanced segregation in strongly segregating alloy systems using recoil sputtering, ion-scattering, SIMS, Auger, XPS, UPS, and LEED techniques. Preparation of controlled stoichiometry high-temperature superconducting films by sequential sputtering of elementary targets.

ARGONNE NATIONAL LABORATORY (continued)

Intense Pulsed Neutron Source Division - 04 -

B. S. Brown - Phone (FTS) 972-5518 or (312) 972-5518

059. INTENSE PULSED NEUTRON SOURCE PROGRAM

B. S. Brown, J. M. Carpenter, A. Rauchas, A. W. Schulke,
T. G. Worlton, R. K. Crawford, F. J. Rotella, C. K. Loong,
P. Thiyagarajan, J. Richardson
Phone: (312) 972-5518

$5,125,000 04-1

Operation and development of IPNS, a pulsed spallation neutron source for condensed matter research with neutron scattering techniques. The facility is equipped with nine instruments which are regularly scheduled for users, two instruments under construction and two beam tubes which are for special experiments or developing instruments. The facility has been run since 1981 as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 230 experiments, involving about 150 outside visitors from universities and other institutions are performed annually. Industrial Research on a proprietary basis, which allows the company to retain full patent rights, has been initiated with a number of companies (e.g., Schlumberger-Doll, Amoco, Sohio, Exxon) and is encouraged. Relevant Argonne research programs appear under the neutron activities of the Materials Science Division of Argonne National Laboratory. An enriched uranium target will be installed that will increase the flux by a factor of three.

060. APS BEAMLINE AND INSERTION DEVICE R & D

G. K. Shenoy, E. E. Alp, S. H. Kim, A. R. Krauss, D. M. Mills,
R. K. Smither, M. G. Strauss, P. J. Viccaro
Phone: (312) 972-5537

$952,000 04-1

Design studies of the components of the insertion devices, beam line, optics, and detectors suitable for 7-GeV Advanced Photon Source. Methodology to calculate the angular distributions and polarization of insertion device radiation. Theoretical calculations of the optical constants and surface reflectances in the 0.5 to 30 keV range for metals and modeling of multilayer optics. Development of a facility to perform photodegradation studies of multilayer optics exposed to high brilliance of future SR sources. Surface segregation methods to produce self-sustaining surfaces of low desorption materials to be used in strategic locations in synchrotron storage rings. Design of a linear CCD/scintillation detector for X-ray range and readout procedures to perform time development studies. Design and construction of a beam line for installation at the Synchrotron radiation Source, Wisconsin, and at the National Synchrotron Light Source - X-ray ring, to carry out angle resolved photoelectron spectroscopy and X-ray scattering studies.

ARGONNE NATIONAL LABORATORY (continued)

061. APS ACCELERATOR R & D

Y. Cho, J. Cook, E. Crosbie, S. Kim, M. Knott, S. Kramer, R. Kustom, G. Mavrogenes, M. Yoon, R. Wehrle, K. Thompson, G. Nicoolls, W. McDowell
Phone: (312) 972-6616

$3,658,000 04-1

Further refinement of the conceptual design of the Advanced Photon Source, new design of a 7-GeV storage ring complex facilitating wide ranges of tunability of insertion devices, and capable of instrumenting about 35 insertion device beamlines compared to 28 insertion device beamlines of 6 GeV design. To illustrate the undulator tunability, when the first and third harmonics of the undulator radiation are utilized, one undulator can cover the photon energy range from a few keV to several tens of keV. The project would start in FY 1989 according to current estimates.

BROOKHAVEN NATIONAL LABORATORY
Upton, NY 11973

M. Blume - Phone (FTS) 666-3735 or (516) 282-3735

Metallurgy and Ceramics - 01 -

A. N. Goland - Phone (FTS) 666-3819 or (516) 282-3819
K. G. Lynn - Phone (FTS) 666-3501 or (516) 282-3501

070. PROGRAM ON STRUCTURE AND PROPERTIES OF SURFACE MODIFIED MATERIALS AND INTERFACES

S. M. Heald, M. W. Ruckman, D. O. Welch, B. Nielsen
Phone: (FTS) 666-2861 or 516-282-2861
$570,000 01-1

Experimental and theoretical studies of the fundamental factors which influence the microstructure and chemical bonding at [redacted]s between dissimilar materials and of surface layers of materials which have been modified by various means to have properties different from those within the bulk of the materials. Systems include metal-metal interfaces, multilayers and grain boundaries. The structural and chemical characterization is carried out using techniques such as glancing angle X-ray reflection and absorption, photoemission, positron annihilation and transmission electron microscopy.

071. FIRST PRINCIPLES THEORY OF HIGH AND LOW TEMPERATURE PHASES

J. W. Davenport, G. Fernando, H. Q. Lin, G. X. Qian, R. E. Watson, M. Weinert, P. Allen (SUNY-Stony Brook)
Phone: (FTS) 666-3789 or (516) 282-3789
$485,000 01-1

Utilization of molecular dynamics and Monte Carlo methods coupled with electronic structure calculations based on the density functional method to study liquids and large unit cell alloys and disordered metals from first principles. Also studies of semiconductor surfaces using molecular dynamics.

BROOKHAVEN NATIONAL LABORATORY (continued)

[illegible] MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS

H. S. Isaacs, A. J. Davenport
Phone: (FTS) 666-4516 or (516) 282-4516
$450,000 01-2

Experimental and analytical studies of passive oxides and surface layers on aluminum, iron and other metals and alloys produced by environmental interactions. Structural and chemical stability of surface films related to corrosion phenomena. Studies of initial stages of formation of surface layers, mechanisms of growth and their breakdown followed by the development of rapid metal dissolution leading to localized corrosion. Studies of the incorportion of corrosion inhibiting anions and the mobility of these ions under existing high electric fields. Dissolution kinetics of metals in highly concentrated electrolytes, salt film formation and diffusion processes. Propagation of transient signals along metal surfaces. Studies of oxide films using EXAFS and EXANES.

073. SUPERCONDUCTING MATERIALS

M. Suenaga, D. O. Welch, R. R. Corderman, Y. Xu, V. Ghosh
Phone: (FTS) 666-3517 or (516) 282-3517
$982,000 01-3

Fundamental properties of high critical temperature and critical field superconductors, mechanical properties, theoretical models of interatomic forces, lattice defects, and diffusion kinetics in superconducting oxides, studies by electron microscopy of lattice defects in superconducting compounds, flux pinning, properties of composite superconductors, new methods of fabricating superconducting materials.

BROOKHAVEN NATIONAL LABORATORY (continued)

CONDUCTOR DEVELOPMENT FOR HIGH T_c SUPERCONDUCTORS

M. Suenaga, S. G. Shyu, Y. L. Wang
Phone: (FTS) 666-3518 or (516) 282-3518
$500,000 01-5

The purpose of this program is to investigate possible methods for fabrication of conductors for dc magnets and ac power transmission lines using the high temperature superconducting oxides such as $YBa_2Cu_3O_7$. The main focus of this program is to measure critical-current densities, J_c, and ac losses of the superconductors which are fabricated by different methods. Also, these materials will be microstructurally characterized in detail and the results will be correlated with the values of J_c and ac losses. The types of conductors which will be investigated are sintered bars and wires and tapes which are fabricated by various methods, e.g., ground powders, polymeric precursors, and aligned polycrystals. Since the wires and tapes will be bonded to substrates, the interdiffusion between the oxides and substrates are also carefully examined for choosing appropriate substrate materials.

Solid State Physics - 02 -

M. Strongin - Phone (FTS) 666-3763 or (516) 282-3763

075. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

S. M. Shapiro, T. Freltoft, A. I. Goldman, Y. J. Uemura, B. Yang, H. Moudden
Phone: (FTS) 666-3822 or (516) 282-3822
$1,157,000 02-1

The principal objective of this program is the fundamental study of structural phase transitions and magnetism by elastic and inelastic neutron scattering. In the area of structural phase transitions, the program emphasizes determination of structural rearrangements and study of dynamical fluctuations in the ordering parameters. The particular emphases are on transformations involving intercalated compounds, systems displaying instabilities at wave vectors which are incommensurate with the lattice, and nonequilibrium effects. The neutron is a unique probe in studying both static and dynamical critical phenomena in magnetic materials. Primary interest is in studies of magnetic ordering, collective magnetic excitations and short-range correlations in all types of magnetic systems. Recent areas of activity involve such systems as La_2CuO_4 and $YBa_2Cu_3O_7$ prototypes of the high T_c superconductors, substitutionally disordered magnetic materials, spin glasses, low-dimensional systems and Martensitic transformations. In addition some complementary muon spin rotation experiments are being performed at the AGS muon beamline.

BROOKHAVEN NATIONAL LABORATORY (continued)

076. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES

G. Shirane, P. Boni, J. Tranquada, L. Rebelsky, K. Yamada, L. Passell
Phone: (FTS) 666-3732 or (516) 282-3732
$1,413,000 02-1

The principal objective of this program is the investigation of the structures and dynamics of ordered and partially ordered condensed matter systems using elastic and inelastic neutron spectroscopy. Currently the lattice dynamics of high T_c superconducting materials is the major area of interest. The program has two other objectives as well: (i) the development and evaluation of new techniques for neutron scattering measurements and (ii) the replacement of certain existing High Flux Beam Reactor (HFBR) instruments with new instruments of improved capability. In regard to the latter category, a polarized neutron, triple-axis spectrometer has been completed as part of a joint US-Japan collaborative program and priority is now being given to the testing of a time-of-flight mode of operation. A prototype spin spectrometer is also being tested.

077. EXPERIMENTAL RESEARCH - X-RAY SCATTERING

J. D. Axe, L. D. Gibbs, B. Ocko, H. D. You
Phone: (FTS) 666-3821 or (516) 282-3821
$1,062,000 02-2

Structural and dynamical properties of condensed matter systems, studied by X-ray and neutron scattering, phase transitions and new states of matter, including two-dimensional (2D) systems, commensurate-incommensurate transformations and surface reconstruction and the structure of buried interfaces. Extension to single crystal interfaces under ultra high vacuum conditions is in progress. X-ray studies of magnetic and magnetoelastic phenomena and the influence of surfaces on phase transformations. New emphasis is on structural phase transformations in high T_c oxide superconductors. Research and development studies of synchrotron instrumentation for NSLS experiments.

BROOKHAVEN NATIONAL LABORATORY (continued)

078. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

K. G. Lynn, R. Mayer, H. Huomo, J. Throwe
Phone: (FTS) 666-3710 or (516) 282-3710
$900,000 02-2

Investigations of perfect and imperfect solids, solid and liquid interfaces and their surfaces by newly developed experimental methods using variable energy positron (.1 eV - 3 MeV) and positronium beams coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron Diffraction, Thermal Desorption Spectroscopy). These tools include two-dimensional angular correlation of annihilation radiation, positronium scattering, positron channeling and diffusion lengths, positron work functions, positronium formation with measurement of its emitted energy distribution on surfaces. Systems that are being studied include metal-metal, polymer-metal and metal-semiconductor interfaces and their alloy formation, strained layer superlattices under various experimental conditions. Bulk positron lifetime and Doppler broadening measurements are being performed on various systems including high temperature superconductors, and some metallic alloys.

079. STRUCTURAL CHARACTERIZATION OF MATERIALS USING POWDER DIFFRACTION TECHNIQUES

D. E. Cox, K. G. Lynn, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516) 282-3818/3870
$338,000 02-2

Application of synchrotron X-ray and neutron powder diffraction techniques to structural analysis of materials, including mixed metal oxides, zeolites, and high T_c superconductors. Phase transition studies at high and low temperatures, including magnetic ordering. High pressure studies in diamond--anvil cells by synchrotron energy-dispersive diffraction techniques. Development of instrumentation and software for powder diffraction analysis. Planning and design of a new high resolution neutron powder diffractometer. Preparation and characterization of bulk samples of inorganic materials, especially high-T_c metal oxide superconductors, including T_c measurements. Orientation and cutting of crystals.

BROOKHAVEN NATIONAL LABORATORY (continued)

080. THEORETICAL RESEARCH

J. W. Davenport, A. Auerbach, P. Bak, V. J. Emery, C. Tang, R. E. Watson, M. Weinert
Phone: (FTS) 666-3789 or (516) 282-3789
$890,000 02-3

Theory of superconductivity in oxides, phase transitions, phenomena in magnetic systems, incommensurate structures, properties of one- and two-dimensional materials by analytical and numerical methods, nonlinear systems, metal surfaces and multilayers, surface states, electronic structure of metals and alloys, using density functional theory, X-ray and neutron scattering, photoemission and inverse photoemission.

081. SURFACE PHYSICS RESEARCH

M. Strongin, P. D. Johnson, S. L. Qui, C. L. Lin, A. Viescas
Phone: (FTS) 666-3763 or (516) 282-3763
$943,000 02-5

Various surface sensitive techniques are used to study the geometrical and electronic properties of surfaces and interfaces. These techniques include LEED, Anger Electron Spectroscopy, Low Energy Ion Scattering, Photoemission, Inverse Photoemission and Spin Polarized Photoemission. Three beamlines covering different photon energy ranges are maintained at the NSLS and form the major part of the program. The research problems include: (a) photoemission and inverse photoemission studies of the electronic structure of metal overlayers, clean metal surfaces and adsorbate covered surfaces; (b) core level photoemission studies of the high T_c superconductors; (c) surface metallurgy and surface compounds; (d) studies of metals embedded in rare gases and solid ammonia at low temperatures; (e) photoemission studies of low temperature oxidation and (g) studies of surface magnetism in thin films and the effect of adsorption on surface magnetism.

BROOKHAVEN NATIONAL LABORATORY (continued)

Materials Chemistry - 03 -

N. Sutin - Phone (FTS) 666-4301 or (516) 282-4301

082. NEUTRON SCATTERING

J. Z. Larese
Phone: (FTS) 666-4349 or (516) 282-4349
$450,000 03-1

The primary objective of the neutron scattering program is the study of phase transitions and critical phenomena in both two and three dimensions. Within this rather broad framework, particular emphasis is placed on molecular films physisorbed on surfaces, martensitic alloys, Rayleigh-Benard convection in $^3He/^4He$ mixtures and oxy-metallates. Most importantly, the detailed information obtained, exploits the unique attributes of the neutron, providing the necessary testing grounds of or stimulus for theoretical models. The combination of both elastic, absorptive, and inelastic techniques represents a method unrivaled in its ability to render a microscopic view of a wide variety of physical phenomena. This points to the fact that both spatial and dynamical information can be readily and often times uniquely recovered in both magnetic and non-magnetic systems.

Engineering Chemistry - 03 -

A. N. Goland - Phone (FTS) 666-3819 or (516) 282-3819
K. G. Lynn - Phone (FTS) 666-3501 or (516) 282-3501

083. SYNTHESIS AND STRUCTURES OF NEW CONDUCTING POLYMERS

T. A. Skotheim, Y. Okamoto, C. Yang
Phone: (FTS) 666-4490 or (516) 282-4490
$503,000 03-2

Development of a fundamental understanding of ionically and electronically conducting polymers and develop techniques for tailoring the materials with highly specific electrical and optical properties. Research consists of the synthesis of new conducting polymers and the exploration of their physical and chemical properties with a number of spectroscopic techniques, including electrochemistry, X-ray absorption spectroscopy, X-ray diffraction, positron annihilation, Fourier transform infrared spectroscopy, and electrical resistivity measurements. The materials of interest are linear polyethers, polysiloxanes, polypyrroles and polythiophenes. The materials are chemically modified by the covalent attachment of electrically active side groups. A second category of materials consists of Langmuir-Blodgett films of polypyrroles and polythiophenes to produce highly ordered two-dimensional structures. This is a collaborative program between Brookhaven National Laboratory, Polytechnic University, University of Lowell and Massachusetts Institute of Technology.

BROOKHAVEN NATIONAL LABORATORY (continued)

High Flux Beam Reactor - 04 -

M. H. Brooks - Phone (FTS) 666-4061 or (516) 282-4061

084. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS

M. H. Brooks, D. C. Rorer, R. C. Karol, L. Junker, J. Petro,
O. Jacobi, T. Prach, R. Reyer, P. Tichler, J. Detweiler, W. Brynda
Phone: (FTS) 666-4061 or (516) 282-4061
$11,000,000 04-1

Operation of the High Flux Beam Reactor, including routine operation and maintenance of the reactor, procurement of the fuel, training of operators, operation and maintenance of a liquid hydrogen moderated cold neutron source, and irradiation of samples for activation analysis, isotope production, positron source production, and radiation damage studies. Technical assistance provided for experimental users, especially with regard to radiation shielding and safety review of proposed experiments. Additionally, planning and engineering assistance provided for projects for upgrading the reactor.

BROOKHAVEN NATIONAL LABORATORY (continued)

National Synchrotron Light Source - 04 -

M. Knotek - Phone (FTS) 666-4966 or (516) 282-4966

085. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT

M. Knotek, S. Krinsky, J. Galayda, J. Godel, J. Hastings, R. Heese, H. Hsieh, R. Klaffky, C. Pellegrini, W. Thomlinson, G. Vignola, G. Williams
Phone: (FTS) 666-4966 or (516) 282-4966

FY88 Materials Sciences Budget: $13,100,000 04-1

The objective of this program is to support operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers operation and maintenance of the two NSLS electron storage rings and the associated injector combination of linear accelerator-booster synchrotron, operation and maintenance of the photon beamlines of the vacuum ultraviolet (VUV) and X-ray storage rings, and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon beam lines of the facility by means of new developments in high resolution photon optics, state-of-the-art monochromators, X-ray mirror systems, detectors, and so on. The NSLS storage rings provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources. While the original design has been solidly based on well developed principles of accelerator technology, this facility is the first in this country to be designed expressly for use of synchrotron radiation, and the objectives in machine performance are quite different from those of importance in high energy physics applications. An extensive research and development (R&D) program is, therefore, necessary in order to optimize performance characteristics and also to develop new beamline instrumentation which will permit users to take full advantage of the unique research capabilities offered by this facility. This R&D effort also supports the construction of the beam lines and devices funded under Phase II construction project.

IDAHO NATIONAL ENGINEERING LABORATORY
EG&G IDAHO, INC.
P.O. Box 1625
Idaho Falls, ID 83415

D. W. Keefer - Phone (FTS) 583-8003 or (208) 526-8003

Metals and Ceramics Unit

R. N. Wright - Phone (FTS) 583-6127 or (208) 526-6127

[redacted] ENTRAPPED HELIUM IN RAPIDLY SOLIDIFIED MATERIAL

R. N. Wright
Phone: (FTS) 583-6127 or (208) 526-6127
$90,000 01-5

Examination of phenomena associated with the interaction of defects with quenched-in helium in rapidly solidified metals. Interactions studied in simple systems to determine fundamental mechanisms. Initial studies made of high-purity aluminum containing ion-implanted helium. Rapidly quenched, high-purity aluminum and dilute precipitation hardening aluminum alloys containing helium examined to study helium interaction with excess vacancies, formation of defect clusters, and microstructural stability. Experimental techniques include positron annihilation and TEM. Atomistic models will be developed.

UNIVERSITY OF ILLINOIS MRL
104 S. Goodwin Avenue
Urbana, IL 61801

H. K. Birnbaum - Phone (217) 333-1370

Metallurgy and Ceramics - 01 -

H. K. Birnbaum - Phone (217) 333-1370

105. TRANSPORT PROCESSES IN LOCALIZED CORROSION

R. C. Alkire
Phone: (217) 333-3640
$ 96,000 01-1

Corrosion of passivating systems. Transport, reaction, and convective diffusion at localized corrosion sites. Initiation at inclusions; corrosion pit growth; corrosion of cracks in static and dynamically loaded systems; corrosion inhibition.

106. DEFECT, DIFFUSION, AND NON-EQUILIBRIUM PROCESSING OF MATERIALS

R. S. Averback
Phone: (217) 333-4302
$275,000 01-1

Ion beam studies of interfaces and diffusion; Rutherford backscattering studies of ion beam effects in solids; crystalline and amorphous transitions; formal properties of nanophase metals and alloys; radiation damage due to ion beams. Development of nanophase ceramics and studies of their physical and mechanical properties. Transport properties and structures of nanophase ceramics are being studied.

107. CENTER FOR MICROANALYSIS OF MATERIALS

J. A. Eades, C. Loxton, J. Woodhouse
Phone: (217) 333-8396, (217) 333-0386, or (217) 333-3888
$118,000 01-1

Chemical, physical and structural characterization of materials. Surface and bulk microanalysis. Electron microscopy, X-ray diffraction, Auger spectroscopy, SIMS and other techniques. Collaborative research programs.

UNIVERSITY OF ILLINOIS MRL (continued)

108. MICROANALYSIS OF DEFECTS AND [redacted]S

J. A. Eades
Phone: (217) 333-8396

$117,000 01-1

Defects, [redacted]ces, segregation are studied by cathodoluminescence and X-ray microanalysis in the transmission electron microscope and by Rutherford backscattering and channeling. Surface convergent-beam diffraction is developed as an analytical technique. An environmental cell for transmission electron microscopy is under construction.

109. GROWTH AND [redacted]T AT METAL AND SEMICONDUCTOR INTERFACES

G. Ehrlich
Phone: (217) 333-6448

$159,000 01-1

Atomic processes important in the growth of crystals and thin films are being characterized on the atomic level using field ion microscopic methods. The diffusivity of single metal atoms will be explored on different planes of the same crystal, as well as on different substrates, in order to establish the importance of structure and chemistry in affecting atomic transport and incorporation.

110. LOCAL STRAIN DETERMINATIONS AT INTERFACES IN METALS AND SEMICONDUCTORS

H. L. Fraser
Phone: (217) 333-1975

$107,000 01-1

Characterization of interfaces in metals and semiconductors using TEM techniques and determining the relationships between the interface structure and properties. Determination of the local state of distortion at strained layer interfaces and at precipitate interfaces in Ni based superalloys is being carried out. The metallurgical engineering of these interfaces is being studied as a means of controlling their properties.

UNIVERSITY OF ILLINOIS MRL (continued)

111. CRYSTAL GROWTH AND PHYSICAL PROPERTIES OF SINGLE CRYSTAL METASTABLE SEMICONDUCTORS

J. E. Greene
Phone: (217) 333-0747

$214,000 01-1

Mechanisms and kinetics of crystal growth. Metastable single crystal alloys for solar and optical applications. Ion-beam sputtering, molecular-beam epitaxy, laser heating and low-energy ion bombardment methods applied to III-V based compounds and III-IV-V_2 chalcopyrite systems.

112. MICROCHEMISTRY OF SOLIDS

C. A. Wert
Phone: (217) 244-0998

$ 16,000 01-1

Development of microanalytic methods for sulfur in coal. Studies of changes in pyrite, pyrrhotite and organic sulfur content during coal treatment and conversion. Internal friction and dielectric loss applications to coal and kerogen structure.

113. PROCESSING AND MICROSTRUCTURE OF COMPLEX CERAMIC SYSTEMS

A. Zangvil
Phone: (217) 333-6829

$187,000 01-1

Microstructure and microchemistry of SiC with covalent additives, such as AlN, BN and BeO; solid solution formation in SiC based systems; effect of processing variables and additives on polytypism and microchemistry. Interfaces and toughening mechanisms in SiC- and mullite-matrix composites. Application of microanalytic methods to analysis of the structure and microchemistry of ceramic high T_c superconductors.

UNIVERSITY OF ILLINOIS MRL (continued)

114. CHEMISTRY OF NEW TRANSITION METAL CERAMIC COMPOUNDS SYNTHESIZED BY MOCVD

G. S. Girolami
Phone: (217) 333-2729

$104,000 01-01

Synthesis of thin film ceramics by chemical vapor deposition method. Studies of the chemistry of precursor compounds at solid surfaces. Preparaiton of transition metal carbides, borides and nitrides using MOCVD methods. Characterization of the microstructures, chemistry, electronic structure, physical properties of the films using a variety of methods. Use of MOCVD methods to develop high T_c superconductor films.

115. SOLUTE EFFECTS ON MECHANICAL PROPERTIES OF [redacted]

H. K. Birnbaum
Phone: (217) 333-1370

$201,000 01-2

Hydrogen effects on deformation and fracture; effects of hydrogen on dislocation mobilities; theoretical model of hydrogen embrittlement; interaction of dislocations with grain boundaries; solute effects on the response of grain boundaries to stress.

116. MICROMECHANICS AND MICROMECHANISMS OF FRACTURE

H. K. Birnbaum, C. J. Altstetter, F. A. Leckie, W. M. Kriven, D. Socie, J. F. Stubbins, I. Robertson
Phone: (217) 333-1370

$ 23,000 01-2

Fracture mechanics and microstructural studies of the fundamental mechanisms of fracture are applied to metals and ceramics. Environmental effects on the fracture of alloys of Fe, Ni, Al, Ti, Al_2O_3-ZrO_2, MgO using HVEM. Role of phase transitions in fracture of hydride forming systems and stainless steels. Effects of environment on dislocation behavior and plasticity related fracture. High-temperature corrosion and scaling. Fatigue and fracture under multiaxial loading and the role of microstructural changes. Development of damage and failure criteria for systems undergoing phase transitions and enhanced plasticity.

UNIVERSITY OF ILLINOIS MRL (continued)

117. COUNCIL ON MATERIALS SCIENCE

C. P. Flynn
Phone: (217) 244-6297

$114,000 01-2

Study and analysis of current and proposed basic research programs on materials and assessment of their relevance to problems of energy utilization. Consideration of national facilities needs. Convening of panel studies on selected topics.

[redacted] MECHANICAL PROPERTIES OF INTERMETALLIC COMPOUNDS

C. Loxton, I. M. Robertson
Phone: (217) 333-0386 or 333-6776

$124,000 01-2

Studies have been made of dislocation/grain-boundary interactions, hydrogen effects and surface oxidation in Ni_3Al. Grain boundaries can pose barriers to slip, causing extensive dislocation pile-ups at the boundary and considerable local elastic strain in the adjacent grain. Strain relief occurs in Ni-rich B-doped material by a sudden and massive generation of dislocations from a length of the boundary into the second grain; in other compositions and in all tests in H atmospheres, strain relief occurs by intergranular failure. Boron appears to enhance boundary cohesion in Ni-rich Ni_3Al and perhaps to facilitate dislocation generation from boundary sources, but only in the absence of H. Oxidation studies indicate the formation of Al_2O_3 at low partial pressures of oxygen (10^{-7} torr); the nature of the phase varies with temperature: phase at 973 K, and an intermediate unstable phase plus an amorphous phase at 773K. At atmospheric pressure the oxide is mixed Al_2O_3 and $NiAl_2O_4$ plus an outer layer of NiO.

119. NEW MECHANISMS OF ENVIRONMENTALLY INDUCED EMBRITTLEMENT

C. J. Altstetter
Phone: (217) 333-4985

$83,000 01-2

Mechanisms of hydrogen related crack growth in stainless steels. Studies over a wide range of hydrogen fugacities and temperature with an emphasis on the mechanisms of fracture. Subcritical crack growth measurements.

UNIVERSITY OF ILLINOIS MRL (continued)

120. HIGH TEMPERATURE TOUGHENING METHODS IN COMPOSITE CERAMICS

W. T. Kriven
Phone: (217) 333-5258

$98,000 01-2

Enhancement of high temperature mechanical properties of multiphase ceramics. Use of high temperature phase transformations of metastable phases to provide toughening at elevated temperature. High temperature mechanical properties of ceramics. Micromechanical measurements of properties. Microcharacterization and microchemistry of phase transformation toughened ceramics.

121. THE ROLE OF DEFORMATION MECHANISMS IN MULTIAXIAL DEFORMATION AND CYCLIC FATIGUE

D. F. Socie
Phone: (217) 333-7630

$73,000 01-2

Behavior of engineering materials subjected top complex loading involving high temperatures, multiaxial state of stress, and time dependent state of stress. Macroscopic damage models are being developed on the basis of microscopic studies of defects accumulated in the materials. High temperature mechanical properties of ceramics under uniaxial, multiaial, and fatigue conditions.

122. MICROMECHANISMS OF FRACTURE

J. F. Stubbins
Phone: (217) 333-6474

$71,000 01-2

Micromechanisms of failure at elevated temperatures under creep, fatigue and aggressive environmental conditions. Role of oxide films on crack initiation and propagation. Microstructural examinaiton of regions in front of cracks and of the dislocation structures are related to micromechanics of failure.

UNIVERSITY OF ILLINOIS MRL (continued)

123. STRUCTURES AND PROPERTIES OF SILICATE GLASSES AND SILICIDE THIN FILMS

H. Chen
Phone: (217) 333-7636

$83,000 01-3

Investigation of the kinetics and mechanisms of thermally induced structural transformation in amorphous silicate glasses and crystalline silicide thin films. Emphasis is placed on the devitrification behavior and silicide layer growth kinetics and interface characterization using X-ray diffraction techniques in an in situ manner.

124. MOLECULAR BUILDING-BLOCK APPROACHES TO CERAMIC MATERIALS

W. F. Klemperer
Phone: (217) 333-2995

$149,000 01-3

Low-temperature synthesis of oxide gels and glasses using a step-wise approach. Polynuclear molecular building-blocks are first assembled and then polymerized into solid materials using sol-gel methods. Silicate cage, ring, and chain alkoxides and their polymerization reactions are studied using multinuclear NMR spectroscopic and gas chromatographic techniques.

[redacted] SYNTHESIS AND PROPERTIES OF DIELECTRIC SOLIDS

D. A. Payne
Phone: (217) 333-2937

$213,000 01-3

Synthesis, powder preparation, crystal growth, forming methods, materials characterization and property measurements on electrical and structural ceramics. Sol-gel processing of thermal barriers and mechanical coatings. Chemical, electrical and mechanical boundary conditions in polarizable deformable solids, twin and domain structures, ferroelasticity and crack propagation. Amorphous ferroelectrics. Synthesis methods and properties of high T_c superconductors.

UNIVERSITY OF ILLINOIS MRL (continued)

126. MICROWAVE STUDIES OF TUNNELING STATES IN DISORDERED MATERIALS

H. J. Stapleton
Phone: (217) 333-0037
$12,000 01-3

Effects of tunneling states and disorder in amorphous semiconductors, fast ionic conductors, glasses, and crystals using electron spin relaxation, electron spin resonance, electron-nuclear double resonance, and microwave susceptibility in the 0.25-25 K temperature range.

127. PROCESSING OF MONODISPERSE CERAMIC POWDERS

C. Zukoski
Phone: (217)-333-7379
$126,000 01-3

Low temperature processing of ceramics including precipitation of monodisperse oxide powders, rheology of monodisperse powders and mixtures, and studies of forces in colloidal suspensions, for the purpose of forming low flaw density, high performance ceramics.

128. ATOMIC SCALE MECHANISMS OF VAPOR PHASE CRYSTAL GROWTH

A. Rockett
Phone: (217) 333-0417
$66,000 01-3

Theoretical studies of the atomic scale processes which determine the surface structures of crystals during vapor phase growth. Monte Carlo imulations of the crystal surfaces including structure and reconstruction of planes with low indices as well as those with high indices. Experimental determination of the surface structure during MBE crystal growth using LEED and RHEED oscillations.

129. RADIATION DAMAGE IN METALS AND SEMICONDUCTORS

I. M. Robertson
Phone: (217) 333-6776
$139,000 01-4

Investigations of vacancy dislocation loop formation and displacement cascades in Fe, Ni, Cu with irradiations and high voltage electron microscopy (at ANL) at 10K to 800K; and of amorphous zones produced in Si, GaAs and GaP by heavy ion irradiation.

UNIVERSITY OF ILLINOIS MRL (continued)

130. ULTRASONIC STUDIES OF RADIATION EFFECTS

A. V. Granato
Phone: (217) 333-2639

$62,000 01-4

Ultrasonic techniques used to determine the basic configuration and dynamics of isolated point defects and their interactions with each other in metals and semiconductors. Studies of paraelastic and dielastic relaxations after electron irradiation in systems such as silicon, GaAs, iron, niobium and aluminum. Measurements over a wide range of temperatures as a function of polarization, frequency, defect concentration, and impurity concentrations.

Solid State Physics - 02 -

H. Zabel - Phone (217) 333-2514

131. LOW-TEMPERATURE STUDIES OF DEFECTS IN SOLIDS

A. C. Anderson
Phone: (217) 333-2866

$100,000 02-2

Experimental studies of glassy metals, of fast ion conductors, of polymers, composites and ceramics, and of irradiated or deformed ionic and other crystals, influence of defects and disorder on macroscopic properties including specific heat, magnetic susceptibility, thermal and electrical transport, thermal expansion, and ultrasonic and dielectric dispersion at 0.02-200K.

132. ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES

T.-C. Chiang
Phone: (217) 333-2593

$158,000 02-2

Synchrotron radiation photoemission studies of electronic properties and growth behaviors of semiconductor surfaces and interfaces prepared in situ by molecular beam epitaxy; properties and atomic structure of alloy surfaces. XPS studies of the band structure of high T_c superconductors.

UNIVERSITY OF ILLINOIS MRL (continued)

133. INVESTIGATIONS OF CRYSTAL GROWTH BY MOLECULAR BEAM EPITAXY

H. Morkoc and C. P. Flynn
Phone: (217) 333-0722
$260,000 02-2

Establishment and operation of a facility for molecular beam epitaxial growth of materials including ceramics, metals and semiconductor single crystals, heterojunction assemblies and superlattices, and for the in situ investigation of epitaxial behavior.

134. PROPERTIES OF CRYSTALLINE AND LIQUID CONDENSED GASES

R. O. Simmons, V. R. Pandharipande
Phone: (217) 333-4170 or (217) 333-8079
$219,000 02-2

Measurement and theory of momentum density in bcc, hcp, and liquid helium, pulsed neutron scattering, phase transitions and structure determination in solid hydrogen by neutron diffraction, isotopic phase separation in solid helium, thermal and isotopic defects in helium crystals, quantum effects in diffusion.

135. NUCLEAR MAGNETIC RESONANCE IN SOLIDS

C. P. Slichter
Phone: (217) 333-3834
$175,000 02-2

Investigations of layered materials and one dimensional conductors with charge density waves, of Group VIII metal-alumina catalysts, and of spin glasses using nuclear magnetic resonance methods. Use of resonance methods to study the role of Cu and O in high T_c superconductivity.

UNIVERSITY OF ILLINOIS MRL (continued)

136. STRUCTURE AND DYNAMICS OF SURFACES, INTERFACES AND HETEROSTRUCTURES

H. Zabel
Phone: (217) 333-2514

$158,000 02-2

X-ray and neutron scattering investigations of structural, thermal and vibrational properties of alkali metal graphite-intercalation compounds, staging, dislocations, point defects, phonon dispersion, order-disorder transformations, and diffusion. Microstructural properties of metal and semiconductor MBE grown superlattices. Studies of high T_c superconductor structures and dynamic properties using scattering methods.

137. THEORY OF SOLIDS, SURFACES, AND HETEROSTRUCTURES

R. M. Martin
Phone: (217) 333-4229

$90,000 02-2

Theoretical studies of the properties of materials using ab-initio calculations in a unified manner. Development of technique applied to known materials and extension of these methods to new materials. Focus on problems involving many bodied correlations of electrons such as high T_c superconductors, surfaces, heterostructures and interfaces.

138. CARRIER TRANSPORT IN QUANTUM WELLS - PICOSECOND IMAGING

J. P. Wolfe
Phone: (217) 333-2374

$37,000 02-2

Development of picosecond imaging techniques applied to measure the lateral transport of photoexcited carriers in semiconductor quantum wells. Optical-pulse-probe methods and spatial imaging techniques applied to GaAs/AlGaAs multilayers. Energy distribution of photoexcited carriers measured with high resolution luminescence imaging methods used to study the scattering processes of carriers and surfaces, interfaces, impurities and phonons.

UNIVERSITY OF ILLINOIS MRL (continued)

Materials Chemistry - 03 -

H. Zabel - Phone: (217) 333-2514

139. PRESSURE TUNING SPECTROSCOPY

H. G. Drickamer
Phone: (217) 333-0025

$158,000 03-1

Studies of the pressure tuning of electronic energy levels with emphasis on optical absorption measurements including absorption edges, metal cluster compounds and charge transfer phenomena, as well as semiconductor-metal interfaces.

140. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS

L. R. Faulkner
Phone: (217) 333-8306

$102,000 03-1

Exciton propagation from absorbing chromophores in polymer films to trapping sites on film surfaces at monolayer coverage. Controlled molecular assemblies of three dimensional reaction systems.

141. OPTICAL SPECTROSCOPY OF SURFACE PROCESSES IN THIN FILM DEPOSITION

E. G. Seebauer
Phone: (217) 333-4402

$35,000 03-1

Surface chemistry during the deposition of GaAs films using LEED, temperature programmed desorption, photoreflection and surface second harmonic generation. The chemistry of the adsorption process and surface diffusion are being probed.

UNIVERSITY OF ILLINOIS MRL (continued)

142. SURFACE STUDIES OF BOUNDARY LAYER FILMS

A. J. Gellman
Phone: (217) 244-5810

$ 92,000 03-1

The long term goal of this program is the understanding of the mechanical properties of interfaces. We will investigate the role of surface structure, and the role of adsorbed species in determining both the adhesive and frictional properties of interfaces between pairs of surfaces. Initial measurements will be made on a macroscopic scale (gram level forces) between pairs of surfaces that have been prepared under vacuum conditions. These will include perfectly clean metal surfaces of varying structure brought together in well defined relative orientations. A second class of interfaces will be formed from surfaces covered with monolayer amounts of adsorbed species. The intention is to study the adsorbate characteristics important in determining mechanical properties, in particular the role of the mode of adsorption. In the first system to be studied we will discriminate between the properties of carboxylic acids adsorbed molecularly or as carboxylate anions.

U of I MRL
$4.614K
+ 25 Univ sal + benefit
≈ $2.5M
= $7.00
+ Similar NSF budget
Maher for $11-12M

LAWRENCE BERKELEY LABORATORY
1 Cyclotron Road
Berkeley, CA 94720

G. Rosenblatt - Phone (FTS) 451-6606 or (415) 486-6606

Materials and Chemical Sciences Division

Norman E. Phillips - Phone (FTS) 451-6063 or (415) 486-6063

Metallurgy and Ceramics - 01 -

145. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES

R. Gronsky
Phone: (FTS) 451-5674 or (415) 486-5674
$176,000 01-1

Transformation interfaces: homophase boundaries, heterophase boundaries, "free" surfaces at which solid-state reactions are either initiated or propagated. Atomic configurations of such interfaces and the relationship between structure and relevant interfacial properties. Transmission electron microscopy, including energy-dispersive X-ray and electron-energy-loss spectroscopies. Correlation with theoretical predictions of interfacial phenomena.

146. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS

G. Thomas
Phone: (FTS) 451-5656 or (415) 486-5656
$502,000 01-1

Fundamental electron microscopic studies of structure-composition-processing-property relationships in metallic, ceramic, magnetic materials. Specific tasks: a) ferrite-martensite steels for rod and wire: microstructure and processing, solute partitioning, fatigue (with Professor R. Ritchie); b) martensitic steels: relation to wear, microalloying; c) electronic magnetic materials: recording media, heads, thin films, and rare-earth permanent magnet alloys.

LAWRENCE BERKELEY LABORATORY (continued)

147. SOLID-STATE PHASE TRANSFORMATION MECHANISMS

K. H. Westmacott
Phone: (FTS) 451-5663 or (415) 486-5663
$176,000 01-1

Factors that govern phase stability in order to facilitate first-principle alloy design. Advanced electron-optical techniques, especially high-voltage and high-resolution electron microscopy. The relationship between lattice defects and precipitate phase growth. Crystallographic theory of precipitation with a parallel experimental program.

148. NATIONAL CENTER FOR ELECTRON MICROSCOPY

G. Thomas
Phone: (FTS) 451-5656 or (415) 486-5656
R. Gronsky
Phone: (FTS) 451-5674 or (415) 486-5674
K. H. Westmacott
Phone: (FTS) 451-5663 or (415) 486-5663
$1,445,000 01-1

Organization and operation of a national, user-oriented resource for transmission electron microscopy. Maintenance, development, and application of specialized instrumentation including an Atomic Resolution Microscope 1.5A point-to-point (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.

149. IN-SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY

J. W. Evans
Phone: (415) 642-3807
$65,000 01-1

Microstructural aspects of reactions between gases and solids. Principal experimental tools are the high-voltage transmission electron microscopy. Environmental cells permit reactions between gases and solids (including oxidation of semiconductor materials) to be observed at full magnification.

LAWRENCE BERKELEY LABORATORY (continued)

150. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS

D. de Fontaine
Phone: (415) 642-8177

$126,000 01-1

Calculations of long-period superstructures in two dimensions using the ANNNI (axial next-nearest-neighbor Ising) model. Experimental elucidation of atomic rearrangements in periodic antiphase structures in Cu_3Pd and Ag_3Mg using atomic resolution and high-voltage electron microscopy.

151. ALLOY THEORY

D. de Fontaine, L. M. Falicov
Phone: (415) 642-8177

$190,000 01-1

The object of this program is to obtain theoretically the temperature-composition phase diagrams of alloys. The approach must combine three different problems into one: (1) accurate band structure calculations; (2) reasonable inclusion of alloy many-body effects; and (3) statistical thermodynamics. Every one of these aspects requires sophisticated theoretical concepts, intensive numerical manipulation, and deep physical insight. Various approximations and computational methods will be tested for each step, and computer codes developed and integrated into a whole, self-consistent algorithm. Important decisions concerning method, input information and desired accuracy must be made all stages. Comparison with experimental data will serve as a guide.

152. HIGH-TEMPERATURE REACTIONS

A. W. Searcy
Phone: (FTS) 451-5900 or (415) 486-5900

$272,000 01-3

Sintering studies with crystalline and glassy oxides using TEM, BET, and weight-loss measurements. Surface thermodynamic theory and theory of time-independent distributions of matter in temperature gradients and application of these theories to sintering and grain growth. Experimental and theoretical studies of solid state reactions.

LAWRENCE BERKELEY LABORATORY (continued)

153. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS

R. H. Bragg
Phone: (415) 642-7393

$75,000 01-3

Kinetics and mechanism of graphitization, i.e., the ordering of carbonaceous precursors when heated in inert atmospheres above 2000°C. Characterization is by wide range X-ray and neutron diffraction, small angle scattering and transmission electron microscopy. Measurements of electronic properties and magnetic susceptibility down to 1.4 K in fields to 6T. Emphasis on the role of carbon interstitials grafted covalently on graphite layer planes.

154. CERAMIC [redacted]

A. M. Glaeser
Phone: (415) 642-3821

$140,000 01-3

Development of model experiments that facilitate investigation of fundamental aspects of microstructural development, and their application of model ceramic systems. Current efforts are directed at: the development of controlled geometry pore arrays at [redacted] in [redacted] for studies of pore coarsening, morphological stability and surface energy anisotropy, the identification of pore-boundary separation conditions in alumina from controlled-pore-structure sapphire-seeded abnormal grain growth studies, the characterization of particle substructure in chemically synthesized titania, and investigation of particle substructure effects on coarsening and sintering behavior of compacts consisting of monosized powders.

Solid State Physics - 02 -

155. FAR-INFRARED SPECTROSCOPY

P. L. Richards
Phone: (415) 642-3027

$194,000 02-2

Improved infrared detectors, mixers, and spectrometers are developed and used in experiments in important areas of fundamental and applied physics. Technological developments include a liquid-helium-cooled grating spectrometer for emission spectroscopy, ultrasensitive photoconductive detectors for the 50-200 μm wavelength range, improved fabrication techniques for bolometric detectors, development of a microcalorimeter for two-dimensional systems and production of tunable picosecond far-infrared pulses by difference frequency generation. Experiments include measurements of the infrared spectra of molecules adsorbed on metal surfaces, and of one-dimensional charge-density wave conductors, measurements of the heat capacity of adsorbed monolayers, measurements of the infrared photoconductivity of impurities in semiconductors, and a test of the Planck theory of thermal radiation with unprecedented accuracy.

156. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS

Y. R. Shen
Phone: (415) 642-4856

$234,000 02-2

Development of linear and nonlinear optical methods for material studies and applications of these methods to probe properties of gases, liquids, and solids. Theoretical and experimental investigation of various aspects of laser interaction with matter are pursued. New nonlinear optical techniques are applied to the studies of isotope separation, photochemistry, molecular clusters, phase transitions, surfaces and interfaces.

LAWRENCE BERKELEY LABORATORY (continued)

157. EXCITATIONS IN SOLIDS

C. D. Jeffries
Phone: (415) 642-3382

$156,000 02-2

One area of study is nonlinear dynamics and instabilities in solid state systems. The objectives are detailed experimental studies of driven plasma instabilities in semiconductors and spin wave instabilities in magnetic materials. These display period-doubling bifurcation, quasi-periodic behavior, and onset of aperiodic noise-like behavior, controlled by a fractal attractor. The observed behavior is compared to various theoretical models. Another area of study is high temperature superconductivity using microwave methods to probe magnetic properties, dynamics of the metastable states, and vortex line instabilities. The project is a basic science effort with results bearing directly on the technology of plasmas, solid state devices, superconductivity, and magnetic materials.

158. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS

P. Y. Yu
Phone: (415) 642-8087

$110,000 02-2

The main objective of this project is to utilize picosecond and subpico-second laser sources to study the ultrafast relaxation processes that occur in semiconductors. The processes under investigation include electron-phonon interactions, phonon-phonon interactions, and electron-electron interactions. The experiments involve exciting dense electron-hole plasmas in semiconductors such as GaAs and monitoring the time evolution of the electron and phonon distribution functions by Raman scattering and photoluminescence. Another area of investigation involves the study of optical properties of semiconductor superlattices, quantum wells and solids under high pressure.

LAWRENCE BERKELEY LABORATORY (continued)

159. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE

J. Clarke
Phone: (415) 642-3069

$234,000 02-2

DC Superconducting Quantum Interference Devices (SQUIDs) developed and used in a wide variety of applications, including geophysical measurements, noise thermometry in the milliKelvin temperature range, and the measurement of electrical noise. An ultralow-noise SQUID amplifier operating at frequencies of up to 200 MHz used to improve the sensitivity of nuclear magnetic resonance and nuclear quadrupole resonance measurements. SQUIDs operating at temperatures down to 20 mK used to study their ultimate noise limitations for such applications as transducers for gravity-wave antennas. Novel experiments to investigate macroscopic quantum tunneling and microwave-induced transitions between quantum states in Josephson tunnel junctions at milliKelvin temperatures. A detailed study of the excess noise induced in metal films by electron bombardment in an electron microscope.

160. QUANTUM THEORY OF MATERIALS

M. L. Cohen, L. M. Falicov, S. G. Louie
Phone: (415) 642-4753

$236,000 02-3

Research to further basic understanding of the physical properties of materials and materials systems such as surfaces and interfaces. Emphasis on carrying out quantum-mechanical calculations on realistic systems so that a microscopic understanding may be obtained from first principles. Studies include bulk materials, surface and chemisorbed systems, interfaces, and defects in solids and clusters. Comparisons with experiment showing that the calculations are accurate and of predictive power. Bulk materials research focused on: electronic, magnetic, structural, and vibrational properties; crystal-structure determination; solid-solid phase transformations at high pressure; and defect properties. Surface and interface research focused and atomic, electronic, and magnetic structures.

LAWRENCE BERKELEY LABORATORY (continued)

Materials Chemistry - 03 -

161. LOW-TEMPERATURE PROPERTIES OF MATERIALS

N. E. Phillips
Phone: (FTS) 451-6063, (415) 486-6063, or (415) 642-4855
$150,000 03-1

Measurements of the low-temperature properties of materials, particularly specific heats, to contribute to the understanding of their behavior. Related work on the temperature scale in the region below 1K where the scale is not well established. Specific heat measurements between 5mK and 100K, at pressures to 20kbar and fields to 9T. Current emphasis is on heavy-fermion compounds, especially heavy-fermion superconductors, and high critical temperature superconductors.

162. ADVANCED CONCEPTS FOR THE PROTECTION OF METALS AND SEMICONDUCTORS

R. H. Muller, J. D. Porter, G. M. Rosenblatt, P. N. Ross, C. W. Tobias
Phone: (FTS) 451-6079 or (415) 486-6079
$120,000 03-2

Basic research aimed at elucidating the role of inhibitors and surface films in the protection of metals and semiconductors from corrosion in agressive environments. Studies to connect detailed processes of adsorption of inhibitor molecules (or ions) and formation of surface films with kinetics of dissolution, rate of evolution of pits, and rate of crack initiation and propagation. Different photon sources used to probe in situ structure of the interface via excitation of molecular vibrations (infrared reflectance, Raman scattering), plasmon excitation (second harmonic generation), and elastic scattering (surface X-ray diffraction). Scanning tunneling microscopy used in situ to study crack (and pit) initiation and the morphological breakdown of surface films.

LAWRENCE BERKELEY LABORATORY (continued)

163. HIGH-TEMPERATURE THERMODYNAMICS

L. Brewer
Phone: (FTS) 451-5946 or (415) 486-5946
$131,000 03-3

Models to predict the behavior of gases, refractory containment materials, and many metallic systems are being developed and expanded. A thermodynamic data compilation for all elements from H to Lr and their oxides in solid, liquid, and gaseous states from 298 to 3000 K is being completed. The main thrust of the experimental program is to provide quantitative predictive models for the strongly interacting alloys exhibiting generalized Lewis Acid-Base behavior. High-temperature solid-electrolyte EMF measurements, vapor pressure measurements, and equilibration with carbides, nitrides, and oxides are being used to characterized the thermodynamics of these systems.

164. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES

D. R. Olander
Phone: (415) 642-7055
$224,000 03-3

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 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. 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 by halogens.

LAWRENCE BERKELEY LABORATORY (continued)

165. NUCLEAR MAGNETIC RESONANCE

A. Pines
Phone: (FTS) 451-6097 or (415) 486-6097
$617,000 03-3

Research on methods in magnetic resonance spectroscopy and study of molecular behavior in condensed phases. Novel techniques developed include multiple quantum spectroscopy, high resolution solid-state NMR, magic angle spinning, zero field NMR, pulsed laser nuclear double resonance for enhanced NMR surfaces, and non-invasive materials imaging. Theoretical topics include iterative mapping, quantum adiabatic phases and 2d NMR studies of molecular dynamics. These methods applied to determination of molecular structure and dynamics, including atomic clustering in condensed matter, in systemssuch as ferroelectrics, liquid crystals, polymers, organic crystals, zeolites, and surfaces. New methods of detection developed to increase the sensitivity of detection, in particular rapidly switched superconducting fields and Josephson juction devices such as SQUIDS.

166. SYNTHESIS OF NOVEL SOLIDS

A. M. Stacy
Phone: (415) 642-3450
$44,000 03-3

Research on new synthetic procedures for the preparation of advanced materials with novel properties. Initial studies focused on transition-metal chalcogenides, since these materials have a variety of interesting electronic properties and uses in energy applications. To overcome the limitations of high-temperature synthetic techniques, procedures involving the modification of various reactants at room temperature are being developed. Such synthetic studies will lead to numerous new classes of materials with novel optical, magnetic, electronic, and surface properties.

LAWRENCE BERKELEY LABORATORY (continued)

Center for Advanced Materials

R. O. Ritchie - Phone (FTS) 451-5798 or (415) 486-5798

[redacted] CAM STRUCTURAL MATERIALS PROGRAM

J. W. Morris, Jr., L. C. DeJonghe, R. O. Ritchie, G. Thomas, T. M. Devine, Jr.
Phone: (415) 486-6482 or (FTS) 451-6482
$1,592,000 01-1

This CAM program focuses on advanced structural materials of interest to American industry. It includes fundamental research on microstructure and mechanical behavior and specific investigations of advanced structural metals and ceramics. It is organized into four projects: (1) Mechanical Behavior (R. O. Ritchie), which addresses the mechanisms of structural failure, including the fatigue and fracture in metals, intermetallics and ceramics; (2) Ceramics (L. DeJonghe), which is focused on the processing of advanced structural ceramics; (3) Metals (J. W. Morris, Jr.), which is concerned with the properties and development of metal alloys, including modern Al-Li alloys for aerospace applications, formable steels for manufacturing, advanced intermetallics, and materials for high field superconducting magnets. Research in the fourth area, structure behavior (A. G. Khachaturyan) involves studies of the theory of microstructure and phase transformations in metals and ceramics and is integrated, as appropriate, into the other sections of the program.

LAWRENCE BERKELEY LABORATORY (continued)

[redacted] CAM ELECTRONIC MATERIALS PROGRAM

Eugene E. Haller, J. Washburn, R. M. Cannon, J. W. Morris, Jr.
Phone: (FTS) 451-5294 or (415) 486-5294
$1,278,000 01-3

Research in this program is focused on material problems impeding the development of advanced electronic devices and device packaging. This includes an integrated crystal growth and characterization effort (E. E. Haller), which seeks an understanding of the incorporation of structural and electronic defects, as well as impurities, during the growth, post-growth annealing, and/or materials processing. Thrust areas including vertical Bridgman crystal growth, formulation of microscopic theories of defect formation in semiconductors, and study of solid phase reactions between the large number of metals and III-V compound semiconductors (J. Washburn). These studies are complemented by comprehensive investigations of structural properties of heterointerfaces. The objective of this research is to improve understanding of the mechanisms of structural defect formation at heterointerfaces and at surfaces modified by ion beams, and also to reveal a correlation between structural defects and electronic properties of heterointerfaces. Additional research addresses the material issues related to the packaging of electronic devices. This includes the study of metallic interconnects for microelectronic devices (J. W. Morris, Jr.). Factors affecting the adhesion between dissimilar materials and aspects of film delamination important for specific practical applications are also investigated (R. M. Cannon).

LAWRENCE BERKELEY LABORATORY (continued)

169. CAM POLYMERS AND POLYMER COMPOSITES PROGRAM

M. M. Denn, D. Theordorou, M. D. Alper
Phone: (415) 642-0176

$703,000 03-2

Development and synthesis of high performance polymeric materials. Currently the program consists of three projects: anistropic polymeric materials, polymer/substrate interactions, and the enzymatic synthesis of materials. The first two are focused on the prediction and control of microstructure during the melt processing of polymeric materials. The first (M. M. Denn) looks primarily at liquid crystal polymers, using rheology, NMR, and structural theory to elucidate how orientation and stress develop during shaping. The way in which the multi-phasic nature of the polymer melts affects macroscopic orientation and orientation rates is of particular concern. The second project (D. Theordorou) emphasizes the theory of polymer conformation and stress state near a solid interface as a means of defining the influence of surface interactions on bulk orientation and stress, and hence on properties. The development of computational methods for predicting structure development and the onset of dynamical instabilities is an integral component of both project areas. The third project (M. D. Alper) seeks to exploit the recent breakthroughs in biotechnology to purify and modify the genes for enzymes and then use those enzymes to polymerize unusual monomers into novel polymers for materials applications.

LAWRENCE BERKELEY LABORATORY (continued)

170. CAM SURFACE SCIENCE AND CATALYSIS PROGRAM

G. A. Somorjai, M. B. Salmeron, A. T. Bell, J. Clarke, T. R. Shen, H. Heinemann
Phone: (415) 642-4053

$1,551,000 03-3

Catalysis research (A. T. Bell, H. Heinemann) is focused on correlating macroscopic catalytic properties of microporous crystalline materials and model single crystal surfaces with their surface structure, chemical bonding and composition. Studies are aimed at understanding the nucleation, growth and structure of zeolites to allow systematic synthesis to carry out specific reactions. Transition metals carbides, oxycarbides, and nitrides are also prepared in microporous crystalline form and characterized. Catalyzed reactions of interest include ammonia synthesis, selective hydrocarbon conversion to produce clean fuels and chemicals and methanol synthesis. The Surface Science effort emphasizes atomic level surface characterization and the relationship between chemical, mechanical, and physical performance and molecular level properties. Included are studies of mechanical and chemical properties of hard coatings (G. A. Somorjai) that are synthesized by plasma deposition and of surfaces at metal-oxide, metal-metal and metal-polymer (organic) interfaces. In an instrumentation project, new techniques and instruments for the study of surfaces and interfaces are developed. Research is focused on scanning tunneling microscopy (J. Clarke, M. Salmeron), nonlinear optical techniques (second harmonic and sum frequency generation) (Y. R. Shen), solid state NMR, and electron and ion scattering spectroscopies (LEED, HREELS, XPS, AES, ISS, SIMS).

LAWRENCE BERKELEY LABORATORY (continued)

171. CAM HIGH-T_c SUPERCONDUCTIVITY PROGRAM

N. E. Phillips, J. Clarke, P. Berdahl, L. C. DeJonghe
Phone: (415) 486-6382

$546,000 02-5

Studies in three major areas: basic science, thin films and their applications, and processing for bulk conductors. Basic science (N. E. Phillips) activities are directed at developing an understanding of the known high-T_c materials in the expectation that it will lead to other materials with superior properties. It includes theoretical work, the synthesis of new materials, growth of single crystals, and the measurement of physical properties (including magnetic susceptibility, transport properties, specific heat, isotope effect, mechanical properties, microwave absorption, electron tunneling, infrared absorption and Raman spectroscopy, and the effect of high pressure on T_c). Theoretical studies include first principles calculations and model-based interpretations of measured properties. Thin films and applications research (J. Clarke) includes fabrication and processing, investigation of physical and electrical properties, development of thin-film devices, including SQUIDS and other applications of Josephson devices, and radiation sensors. It also includes a Thin Films Information Center (P. Berdahl). Processing research (L. C. DeJonghe) is directed at understanding and overcoming problems in producing high-current capacity conductors, identification of sintering mechanisms, examination of the effects of the powder calcination conditions on microstructure and twinning, carbon-free processing, consideration of grain-boundary chemistry, evaluation of factors limiting critical current densities as well production of grain-oriented bulk materials and characterization of their electrical and microstructural properties.

Accelerator and Fusion Research Division

K. Berkner - Phone (FTS) 451-5501 or (415) 486-5501

172. R&D FOR ADVANCED PHOTON SYSTEMS

M. R. Howells, J. H. Underwood, D. T. Attwood
Phone: (FTS) 451-4949

$873,000 02-2

The synchrotron radiation community is now on the threshold of developing a new generation of X-ray facilities that will produce radiation which is extremely bright, powerful, and in some cases partially coherent. In the past, this program has addressed design studies of next-generation undulators and the design and fabrication of high-thermal-loading beamline hardware. Current activities focus on the design, fabrication, commissioning, and operations support of beamlines and beamline components at SSRL and NSLS.

LAWRENCE BERKELEY LABORATORY (continued)

173. CENTER FOR X-RAY OPTICS

D. Attwood
Phone: (FTS) 451-4463 or (415) 486-4463
$1,169,000 02-2

The Center for X-Ray Optics focuses on the development of technologies required for the utilization of emerging sources of XUV radiation in applications to science and industry. The Center has organized laboratories and collaborations that have led to the development and broad utilization of new technologies for the production, efficient transport, focusing, dispersion and detection of radiation with photon energies extending from several eV to many keV. Studies have included the development of coherent XUV radiation sources based on modern electron storage rings and the use of permanent-magnet periodic structures. The activities of the Center have the common goal of extending the use of XUV radiation for basic and applied research.

174. 1-2 GeV SYNCHROTRON LIGHT SOURCE R&D

J. N. Marx, R. B. Yourd
Phone: (FTS) 451-5244 or (415) 486-5244
$2,000,000 04-1

Answering the national need for a 1-2 GeV synchrotron light source, the Advanced Light Source will be a next-generation source in which high spectral brightness is achieved by a combination of long magnetic insertion devices (wigglers and undulators) driven by a low-emittance electron beam in the storage ring. R&D activities include accelerator physics studies of effects of multiple insertion devices, conceptual studies of feedback control of instabilities, and general consultation related to the basic concepts underlying the injector and storage ring, and development of engineering models of critical components for the injector, storage ring, and beamlines.

LAWRENCE LIVERMORE NATIONAL LABORATORY
P. O. Box 808
Livermore, CA 94550

T. Sugihara - Phone (FTS) 543-8351 or (415) 423-8351

190. SYSTEMATICS OF PHASE TRANSFER IN METALLIC ALLOYS

L. Tanner
Phone: (415) 423-2653

$345,000 01-1

Investigations of the systematics of liquid-to-solid and solid-to-solid phase transformations in metallic alloys. Bulk and surface processing by rapid quenching produce stable and metastable crystalline phases from the melt. Thermal, mechanical and irradiation treatments are being used to transform one crystalline phase to another or to the metallic glass state. Characterization of microstructures by X-ray diffraction, optical and electron microscopy and high-resolution TEM. Correlation of results with current thermodynamic and kinetic models for solidification, solid-state amorphization and martensitic transformations.

191. METASTABLE ALLOY SURFACES PRODUCED BY DIRECTED ENERGY LASERS, ELECTRON AND ION BEAMS

E. N. Kaufmann, J. S. Huang
Phone: (415) 423-2640

$180,000 01-1

Investigations of microstructures produced in alloy layers created by rapid heating and cooling via electron- or laser-beams and by atomic mixing via ion-beams. Studies of the dependence of crystalline phase and glass formation as a function of binary phase relationships, epitaxial relationships, and resolidification velocity. Studies of the morphology of layers formed from film-on-substrate and bulk alloy starting geometries. Comparisons of laser- and electron-beam processing modes. Analysis using electron microscopy, optical microscopy, X-ray diffraction, Auger and ion-beam spectroscopies, as well as computer simulation of the processes.

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

192. OPTICAL MATERIALS RESEARCH

L. L. Chase, S. Payne, H. Lee, N. Winter
Phone: (415) 422-6151

$737,000 02-2

New optical materials suitable for active laser media or transmitting optics in high-power laser systems are prepared and characterized. Properties measured include absorption and emission spectra and cross-sections, lifetimes, nonlinear refractive index, and nonlinear absorption. Ab initio theoretical calculations of energy levels and optical properties of ion-host systems are performed. Physical and chemical mechanisms for optical surface damage are investigated using spatially and temporally resolved photo-emission of electrons and ions, time-of-flight mass spectroscopy, and surface chemical analysis.

LOS ALAMOS NATIONAL LABORATORY
P. O. Box 1663
Los Alamos, NM 87545

F. A. Morse - Phone (FTS) 843-1600 or (505) 667-1600

Metallurgy and Ceramics

D. M. Parkin - Phone (FTS) 843-8455 or (505) 667-8455

200. IRRADIATION-INDUCED METASTABLE STRUCTURES IN CERAMICS AND HIGH-TEMPERATURE SUPERCONDUCTORS

F. W. Clinard, Jr.
Phone: (505) 667-5102

$305,000 01-4

Metastable and topologically-disoriented structures produced in ceramics and oxide superconductors by nuclear (neutron, fission fragment, and alpha-recoil) and charged particle irradiation. Thorium silicate and Cu-O based superconductors. Effect of irradiation temperature, damage rate, particle mass, and energy. Role of nonstoichiometric displacement ratios. Common effects and intrinsic differences in damage response and recovery mechanisms for these materials. Role of starting composition and crystal structure. Evolution of the amorphous state, localized and global disorder, and crystallization. Modeling of damage microstructures and their dependence on damage rate and temperature. Implications for the effect of non-irradiation-induced defects on physical properties. Characterization by X-ray and electron diffraction, electron microscopy, EXAFS, dilatometry, calorimetry, resistivity, superconducting transition temperature, critical current, critical field, and Meissner effect.

LOS ALAMOS NATIONAL LABORATORY (continued)

[redacted] MECHANICAL PROPERTIES

M. G. Stout, U. F. Kocks, R. B. Schwarz, T. E. Mitchell
Phone: (505) 667-4665
$830,000 01-5

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes, Bauschinger effects. Characteristics of and mechanisms controlling the large strain deformation of aluminum, nickel, copper, brass, substructural and textural evolution with strain, strain state, and strain rate. Predictions of texture evolution using crystal plasticity and strain-rate sensitivity. Kinetics of plastic flow at room and elevated temperatures. Response of metals to high strain rates, Hopkinson split-pressure bar experiments dislocation dynamics, threshold stress at 0 K, viscous drag. Dynamics of microstructural evolution. Synthesis and characterization of amorphous alloys. Study of phase equilibria, transformation kinetics of solid-state amorphizing reactions, mechanical alloying, sintering dynamic compaction. Characterization of atomic structure, thermal stability resistance to oxidation and corrosion, magnetic susceptibility. Study of the microstructure, texture, and dislocation structure of high Tc and perovskites texture development and bulk compaction of high Tc ceramics.

202. STRUCTURAL CERAMICS

D. S. Phillips, T. N. Taylor, K. C. Ott, P.D. Shalek,
J. L. Craig
Phone: (505) 667-5128
$345,000 01-5

Mechanistic studies of crack propagation in model SiC-whisker reinforced glass matrix composites. Identification and modification of indigenous whisker surface species with implications for both mechanism and magnitude of toughening from crack tip-whisker interaction. Photoelastic characterization of both local and long-range stress fields resulting from whisker incorporation, crack incorporation, and crack-whisker interaction.

LOS ALAMOS NATIONAL LABORATORY (continued)

Solid State Physics - 02 -

D. M. Parkin - Phone (FTS) 843-8455 or (505) 667-8455

203. CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY

R. Pynn
Phone: (505) 667-6069

$2,088,000 02-1

Research in condensed matter science using the pulsed spallation neutron source at the Los Alamos Neutron Scattering Center (LANSCE). Topics of current interest include collective excitations such as magnons and phonons, single-particle excitations in quantum solids and liquids, molecular vibrations, surface-adsorbed species and hydrogen modes in metals, high-temperature superconductors, f-electron systems, metallic glasses, metallurgical problems in the actinides, and metal hydrides. Staff members also interact, often collaboratively, with researchers from other programs at Los Alamos, as well as from various outside institutions, on a broad range of neutron scattering applications in materials science, chemical physics, crystallography, and structural biology.

204. MATERIALS UNDER EXTREME CONDITIONS

R. LeSar, D. Schiferl, D. Taylor, J. W. Shaner
Phone: (505) 665-0420

$230,000 02-2

Studies of solidification, crystal structures, phase transformations, and thermodynamics of simple molecular systems from low to high temperatures (10 to 1300K) in high-pressure diamond anvil cells (DACs) (up to 500 Kbar) using UV, IR, Mossbauer, and Raman spectroscopy and laser-beam, neutron, and X-ray scattering. Develop theories of phase transformations, structural behavior, and chemical reaction kinetics. Use DACs to prepare and characterize exotic materials, including rare-gas and hydrogen-containing molecules. Study molecular crystal/metallization transformations. Develop high-temperature diamond anvil cell technology, including refractory metal alloys for cell components.

LOS ALAMOS NATIONAL LABORATORY (continued)

205. CORRELATED ELECTRONS IN METALS

Z. Fisk, J. D. Thompson, A. Arko
Phone: (505) 667-0892

$240,000 02-2

Experimental and theoretical investigations of the electronic, magnetic and superconducting properties of binary and ternary alloys, compounds and oxides with highly-correlated electrons. Studies of exotic properties in heavy Fermion, high Tc oxide and other narrow-band materials, including valence and spin fluctuations, crystallographic instabilities, catalytic behavior, unconventional magnetism and superconductivity. Experimental techniques include susceptibility, resistivity, specific heat, ultrasound, crystallography, muon spin rotation, neutron scattering and sample preparation, chemical and structural characterization. Environments are pressures to 50 GPa, temperatures from 0.01 to 300 K and magnetic fields to 20 T.

206. INVESTIGATIONS OF SUPERCONDUCTORS WITH HIGH CRITICAL TEMPERATURES

J. L Smith
Phone: (505) 667-4476

$500,000 02-5

This project is a collaborative effort with ORNL and LBL on the investigation of high-temperature oxide superconductors. The efforts will focus on synthesis of new materials, characterization and analysis, thin films, high current conductors, and oxygen isotopes.

207. THERMAL PHYSICS: NONLINEAR, NONEQUILIBRIUM BEHAVIOR OF MATERIALS/HEAT ENGINES

G. W. Swift, R. Ecke
Phone: (505) 665-0640

$297,000 02-5

Natural or intrinsically irreversible engines: acoustic engines using liquids, gases, and superfluids, heat pumps and prime movers; acoustic turbulence; liquid propylene heat engine: regenerators, heat exchangers, mechanicals, seals; thermal convection in dilute solutions of ^3He in superfluid ^4He near 1 K: steady and oscillatory, nonlinear dynamics and chaos, NMR, microtomographic and optical shadowgraph imaging; superfluid liquid ^3He: A --> B phase transition dynamics.

LOS ALAMOS NATIONAL LABORATORY (continued)

Materials Chemistry - 03 -

D. M. Parkin - Phone (FTS) 843-8455 or (505) 667-8455

208. CONDUCTING POLYMERS AS SYNMETALS

M. Aldissi, A. R. Bishop, D. K. Campbell, B. S. Jorgensen
Phone: (505) 667-1326

$278,000 03-2

Investigation of synthesis-structure-property relations are studied by iterative application of rigorously controlled synthesis of conducting polymers, detailed physical and chemical characterization of their properties, and detailed theoretical modeling and comparisons with a spectrum of materials and experimental data. Polyacetylene and other analog materials are studied as a class, investigating new synthesis and controlled doping methods.

209. ORIGINATING SUPER-STRONG LIQUID-CRYSTALLINE POLYMERS

F. Dowell, R. Liepins, B. C. Benicewicz
Phone: (505) 667-8765

$570,000 03-2

This is a basic research project to originate the next generation of liquid-crystalline polymers (LCPs)--i.e., an entirely new class of LCPs whose strength characteristics are exceptionally superior both in magnitude and dimensionality to present LCPs. Super-strong LCPs are designed to have exceptional strength in three dimensions on a microscopic, molecular level in order to make the first super-strong LCP fibers, thin films, and bulk materials. We have made substantial progress in the origination of theories for LCPs (and resulting transfer of this new theoretical technology to industry and academia), the theoretical design of candidate super-strong LCPs, the chemical synthesis of these new LCPs, and the preparation for their experimental characterization. The new theories and chemical synthesis techniques test very well on existing LCPs and other existing materials.

LOS ALAMOS NATIONAL LABORATORY (continued)

210. LANSCE OPERATIONS SUPPORT, SPECTROMETER DEVELOPMENT, AND USER SUPPORT

R. Pynn
Phone: (505) 667-6069

$1,700,000 04-1

There are continual gains to be made in neutron production by optimization of the LANSCE target/moderator/reflector system. In particular, the moderating systems must be matched to the needs of neutron spectrometers by selection of appropriate materials, geometry, and operating temperatures. The intense neutron flux at LANSCE will provide higher data rates then have ever been seen before from the neutron scattering instruments. To meet this need, we have developed a new generation of ultra-fast computer-based data acquisition systems using the international standard FASTBUS framework. To make optimum use of the source characteristics made available by the PSR and the advanced target/moderator system, suitable time-of-flight spectrometers are required. During the next three to four years, several new spectrometers will be installed at LANSCE, including: a chopper spectrometer for inelastic scattering measurements and Brillouin scattering; a neutron reflectometer with a polarized-neuton option; and a back-scattering spectrometer with a resolution of 10 μeV or better. A national user program requires LANSCE support personnel to assist in the operation of the instruments and to familiarize users with the operation of the facility. A scientific coordination and liaison office has been established with responsibility for dissemination of information about the facility and the coordination of the user program.

OAK RIDGE NATIONAL LABORATORY
P. O. Box 2008
Oak Ridge, TN 37831

B. R. Appleton - Phone (FTS) 624-4321 or (615) 574-4321

Metallurgy and Ceramics - 01 -

J. O. Stiegler - Phone (FTS) 624-4065 or (615) 574-4065

[redacted] THEORETICAL STUDIES OF METALS AND ALLOYS

W. H. Butler, C. L. Fu, G. S. Painter, G. M. Stocks,
Nancy F. Wright
Phone: (615) 574-4845

$806,000 01-1

Use of density functional theory to calculate the properties of materials. Use of KKR-CPA to calculate such properties of alloys as phase diagrams, thermodynamic properties, magnetic properties, lattice constants, short-range order parameters, electrical and thermal resistivities. Use of high-speed band theory (FLAPW, LMTO and QKKR) to calculate total energies of metals and intermetallic compounds. Calculation of properties of surfaces and interfaces. Calculation of electron-phonon interactions, electrical resistivities and superconducting properties for metals and alloys. Use of density functional theory and LCAO method to calculate the properties of clusters of atoms. Application of cluster calculations to materials problems such as impurity effects, grain boundary cohesion and grain boundary segregation. Calculation of structures and properties of oxides and high T_c superconductors.

221. X-RAY RESEARCH USING SYNCHROTRON RADIATION

C. J. Sparks Jr., G. E. Ice, L. D. Specht
Phone: (615) 574-6996 ORNL, (516) 282-5614 NSLS

$592,000 01-1

Use of synchrotron radiation as a probe for the study of metal alloy and ceramic systems. Emphasis on the ability to select a particular X-ray energy from the synchrotron radiation spectrum to selectively highlight specific elements. Thus, the atomic arrangements among the various elements forming the materials can be unraveled and related to the materials' physical and chemical properties. Have operational X-ray beam line on the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. Important materials' problems under study include: (1) effects of short-range order among atoms on radiation induced swelling and mechanical behavior and atomic displacements, (2) studies of the distribution of vacancies and other defects associated with nonstoichiometry and element substitution in long-range ordered alloys which affect ductility, ordering temperature and phase stability, (3) structural changes accompanying ion implantation, surface and interface structures.

OAK RIDGE NATIONAL LABORATORY (continued)

[redacted] MICROSCOPY AND MICROANALYSIS

J. Bentley, D. C. Joy, E. A. Kenik, M. K. Miller
Phone: (615) 574-5067

$867,000 01-1

Development and application of analytical electron microscopy (AEM) and atom-probe field-ion microscopy (APFIM) to determine the microstructure and microchemistry of materials. Equilibrium and radiation-induced segregation at grain boundaries and interfaces by APFIM/AEM, correlation of GB structure and segregation. Radial distribution function determination by EXELFS and electron diffraction intensity profiles. APFIM/AEM studies of high T_c superconductors. Lattice site location in alloys by electron channeling microanalysis. APFIM characterization of modulated structures, spinodals, early stages of phase transformations, and irradiated pressure vessel steels. GB phases and segregation in structural ceramics, ion-implanted ceramics, SiC creep, boron segregation and dislocations in Ni_3Al, short and long-range order in Ni_4Mo.

[redacted] RADIATION EFFECTS

L. K. Mansur, R. A. Buhl, R. E. Clausing, K. Farrell,
L. Heatherly, Jr., E. H. Lee, M. B. Lewis, N. H. Packan,
D. F. Pedraza, R. E. Stoller
Phone: (615) 574-4797

$1,317,000 01-4

Theoretical and experimental research on defects and microstructures produced by irradiation, ion beam treatment and other processes. Principles for design of improved materials. Studies using multiple simultaneous ion beams. Ion beam modification of phase relationships and surface-sensitive mechanical properties; new materials by ion beam processing. Neutron damage in pure metals, alloys, and ceramics irradiated in HFIR, EBR-II and FFTF. Effect of alloying additions; impurities and microstructure on dimensional instability and embrittlement; phase stability under irradiation; relationship between ion and neutron damage; effect of helium and other impurities on microstructure and microcomposition; theory of microstructural evolution based on defect reactions; Fe, Al, Zr, Ni, and austenitic Fe-Cr-Ni alloys; ferritic alloys; MgO, Al_2O_3, $MgAl_2O_4$.

OAK RIDGE NATIONAL LABORATORY (continued)

[redacted] HIGH TEMPERATURE ALLOY DESIGN

C. T. Liu, M. H. Yoo, J. H. Schneibel, W. C. Oliver,
J. A. Horton, W. D. Porter, E. P. George
Phone: (615) 574-4459

$1,275,000 01-5

Design of ordered intermetallic alloys based on Ni_3Al and other aluminides (e.g., $TiAl_3$). Study of the effect of alloy stoichiometry on structure and properties of grain boundaries, nature and effects of point defects, and microalloying and grain-boundary segregation. Study of superlattice dislocation structure, solid-solution hardening, mechanistic modeling of anomalous temperature dependence of yield stress, and deformation and fracture behavior of aluminides in controlled environments at elevated temperatures. Study of superplastic behavior, grain-boundary cavitation, and theoretical modeling of creep behavior of Ni_3Al alloys. Study of the effect of electron structure and atomic bonding on both intergranular and transgranular fracture (e.g., cleavage). Experimental work on structure and properties of aluminide materials prepared by conventional methods and innovative processing techniques. Establishment of correlation between mechanical properties, microstructural features, and defect structures in aluminides.

225. TOUGHENING AND RELATED PROCESSING MECHANISMS IN CERAMICS

P. F. Becher, P. Angelini, A. Bleier, C.-H. Hsueh
Phone: (615) 574-5157

$940,000 01-5

Experimental and theoretical approaches are being developed to provide new insights into mechanisms which improve the toughness, strength, and elevated temperature mechanical performance of ceramics with companion studies in ceramic processing leading to controlled densification, microstructures and compositions, in such toughened systems. The pertinent micro- and macroscopic characteristics are directly related to phenomena that are controlled during powder synthesis, powder processing, and densification. Thus, this task incorporates interdisciplinary studies of the fundamental descriptions of powder synthesis and processing and their influence on densification mechanisms and microstructure evolution during densification. These are directly coupled with studies of the role of microstructure, composition, and defects in the mechanical behavior of ceramics and descriptions of toughening-strengthening and related mechanisms. A primary consideration of these studies is providing the fundamental insights for design and fabrication of ceramics and ceramic composites (e.g., transformation and second phase toughening behaviors).

OAK RIDGE NATIONAL LABORATORY (continued)

226. FUNDAMENTALS OF WELDING AND JOINING

S. A. David, J. M. Vitek
Phone: (615) 574-4804

$490,000 01-5

Correlation between solidification parameters and weld microstructure, distribution, and stability of microphases, microstructure of laser-produced welds, hot cracking, modeling of transport and solidification phenomena in welds, structure-property correlations, austenitic and ferritic stainless steels, electron beam welding, American Welding Institute (AWI), university collaborations.

227. STRUCTURE AND PROPERTIES OF SURFACES AND [redacted]

C. J. McHargue, P. S. Sklad, M. B. Lewis, R. A. McKee, F. A. List
Phone: (615) 574-4344

[redacted] 01-5

Structure of ion-implanted Al_2O_3, SiC, and TiB_2 by backscattering-channeling and TEM, hardening, surface fracture toughening and wear of ion-implanted ceramics, structure and properties studied as a function of implantation parameters (temperature, fluence, energy, ion species) and annealing (temperature and environment). Mechanical behavior of thin films and [redacted], stress relaxation and dissipation. Adherence of oxide and metal films. Ion beam mixing and amorphization of multi-layer metallic alloys and ceramics. [redacted] growth of layered ceramics.

OAK RIDGE NATIONAL LABORATORY (continued)

Solid State Division - 02 -

F. W. Young - Phone (FTS) 624-6151 or (615) 574-6151

228. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS

R. M. Moon, J. W. Cable, H. R. Child, J. Fernandez-Baca, M. Hagen, J. B. Hayter, H. A. Mook, R. M. Nicklow, H. G. Smith, Phone: (615) 574-5234

$1,035,000 02-1

Inelastic neutron scattering studies of phonons, magnons, and single-particle excitations in condensed matter, elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials, lattice dynamics of NiAl, I_2, Sm, Li, and In-Tl alloys, magnetic excitations in amorphous systems, paramagnetic Ni, Fe, Gd, Sm, Tm, $HoFe_2$, and $RbCoF_3$, phase transitions in Ni_3Mn, Cu(Fe), Li, Na, $CsMnBr_3$, and random-field systems, nuclear spin ordering in Pr, $PrCu_2$, and $Cs_2NaHoCl_6$, momentum distributions in ^3He and ^4He. New research directions will include more emphasis on materials properties under extreme environments of high pressures, high temperatures, or ultralow temperatures.

229. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES

R. M. Moon, J. W. Cable, H. R. Child, J. Fernandez-Baca, J. B. Hayter, H. A. Mook, R. M. Nicklow, H. G. Smith, S. Spooner, G. D. Wignall
Phone: (615) 574-5234

$690,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors and metal hydrides, and defects in single crystals, lattice dynamics and UBe_{13}, phase transitions in Mn-Cu alloys, $CoCr_2O_4$, ZrO_2, heavy fermion superconductors, high-T_c superconductors and reentrant superconductors, SANS from ferrofluids, micelles under shear, polymers and polymer blends, metal alloys, liquid crystals and biological systems, kinetics of first-order phase transitions.

OAK RIDGE NATIONAL LABORATORY (continued)

230. SUPPORT FOR NEUTRON USERS' PROGRAM

R. M. Nicklow, J. W. Cable, H. R. Child, J. Fernandez-Baca,
H. A Mook, R. M. Moon, H. G. Smith
Phone: (615) 574-5240

$595,000 02-1

ORNL neutron scattering facilities are available to outside scientists through Neutron Users' Program. Recent investigations include lattice dynamics and magnetic properties of intercalated graphite, NiAl, LiAl, structure and dynamics of spin glasses, random field systems, polarized-beam studies of paramagnetism, heavy fermion superconductors, quasicrystals, amorphous magnetic materials, proton diffusion in biological systems, and collagen periodicity in bones. New facilities include a high-resolution powder diffractometer and a four-circle single-crystal diffractometer with a cryostat for low-temprature crystallography studies.

231. PHYSICAL PROPERTIES OF ADVANCED CERAMICS

J. B. Bates, F. A. Modine, S. T. Sekula, C. Y. Allison,
D. K. Christen, Y. T. Chu, N. J. Dudney, G. R. Gruzalski,
E. Sonder, J. R. Thompson, J. C. Wang
Phone: (615) 574-6280

$1,380,000 02-2

Physical and chemical properties of advanced ceramics including single-phase and composite materials as well as solid-solid interfaces and surface-modified materials. Included in the investigations are refractory materials such as transition metal carbides and nitrides; solid ionic conductors such as silver halide-aluminum oxide composites, beta-alumina, and stabilized zirconia; electronic materials such as zinc oxide and high T_c superconducting oxides; and surface modified and interface structures such as amorphous alumina on single crystal aluminum oxide and metal-electrolyte interfaces. Electrical, dielectric, magnetic, and optical properties, impurity diffusion, defect structure, phase segregation, effects of high temperature and irradiation are emphasized. Techniques include impedance spectroscopy, transient signal analysis, small-angle neutron and micro-Raman scattering, infrared attenuated total reflectance, dc magnetization, ac magnetic response, ion and fast neutron irradiation, model calculations and computer simulations.

OAK RIDGE NATIONAL LABORATORY (continued)

232. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION

D. H. Lowndes, D. J. Eres, D. B. Geohegan, G. E. Jellison,
D. N. Mashburn, S. J. Pennycock, R. F. Wood
Phone: (615) 574-6306

$990,000 02-2

Picosecond laser spectroscopy, time-resolved reflectivity, transmissivity, and ellipsometric measurements, time-resolved transient electrical conductivity, light-assisted chemical vapor deposition of thin films, modulated layered structures, and superlattices, fabrication of superconducting thin films by laser ablation, laser-induced recrystallization of amorphous layers, thermal and laser annealing of lattice damage in Si, Ge, and GaAs, fabrication of high-efficiency solar cells by laser techniques, investigations of thermo-photovoltaic systems, effects of point defects, and impurities on electrical and optical properties of single-crystal and polycrystalline Si, electrical, optical (including infrared and luminescence spectroscopy), transmission electron microscopy, X-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering measurements, dopant concentration profile, deep-level transient spectroscopy, and absolute quantum efficiency measurements.

OAK RIDGE NATIONAL LABORATORY (continued)

233. SYNTHESIS AND PROPERTIES OF NOVEL MATERIALS

L. A. Boatner, M. M. Abraham, Y. K. Chang, C. B. Finch,
J. O. Ramey, B. C. Sales
Phone: (615) 574-5492

$1,167,000 02-2

Preparation and characterization of advanced materials including the growth of single crystals and the development of new crystal growth techniques; development of new materials through the application of enriched isotopes; investigations of the physical, chemical, and thermal properties of novel materials using the techniques of thermal analysis, X-ray diffraction, Mossbauer spectroscopy, ion implanation and ion channeling, optical absorption, high performance liquid chromatography, EPR, and neutron scattering; application of materials sciences techniques to the resolution of basic research problems; preparation and characterization of high T_c superconducting oxides; synthesis and investigation of phosphate glasses; development and characterization of advanced ceramics; studies of solid state epitaxial regrowth; rf-induction growth of transition-metal carbides; growth of perovskite structure oxides, high-temperature materials (MgO, CaO, Y_2O_3), refractory metal single crystals (Ir, Nb, Ta, V), fast ion conductors, stainless steels.

234. SMALL-ANGLE X-RAY SCATTERING

G. D. Wignall, J. S. Lin, S. Spooner
Phone: (615) 574-5237

$163,000 02-2

Small-angle X-ray scattering of metals, metallic glasses, precipitates, alloys, polymers, and surfactants, fractal structures in polymers and oxide sols, surface modification under ion bombardment, domain structures in composites, dynamic deformation studies of polymers, time-slicing studies of phase transformation. Facilities are available to users through National Center for Small-Angle Scattering Research (NCSASR).

OAK RIDGE NATIONAL LABORATORY (continued)

235. THEORY OF CONDENSED MATTER

J. F. Cooke, J. H. Barrett, H. L. Davis, R. Fishman, T. Kaplan, S. H. Liu, G. D. Mahan, M. E. Mostoller, O. S. Oen, M. Rasolt, M. T. Robinson, J. C. Wang, R. F. Wood, D. Zimmerman
Phone: (615) 574-5787

$1,210,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors, lattice vibrations in metals and alloys, lattice dynamics and potential energy calculations of ionic crystals, computer simulation of radiation damage, sputtering, and ion implanation surface studies with backscattered ions, development of LEED theory and interpretation of LEED data, surface vibrations and relaxation, electronic structure of metal surfaces, magnetism in transition metals and local moment systems, electronic properties of mixed-valent and heavy fermion systems, critical phenomena and phase transitions quantum Hall effect, diffusion and elastic vibrations of fractal systems. New directions include: neutron scattering at high energies, surface structure of alloys, basic mechanism and phenomenology of high-temperature superconductivity.

[redacted] X-RAY DIFFRACTION AND ELECTRON MICROSCOPY

B. C. Larson, J. D. Budai, M. D. Galloway, S. Pennycook, J. Z. Tischler
Phone: (615) 574-5506

$1,068,000 02-4

Microstructure and properties of defects in solids, transmission electron microscopy, synchrotron X-ray scattering, time-resolved X-ray scattering, X-ray diffuse scattering, X-ray topography, neutron and ion irradiation induced defect clusters in metals, pulsed-laser-induced melting and crystal growth, enhanced diffusion in semiconductors, defects associated with laser and thermal processing of pure and ion-implanted semiconductors, grain boundaries in semiconductors, high-resolution atomic imaging of defects, direct imaging and microscopic lattice location of dopants in semiconductors, solid-phase recrystallization in semiconductors, structure of high-temperature metal carbides, anisotropic elastic theory of dislocation loops, computer simulation of electron microscopy images, development of analytical techniques of electron microscopy, calculation of diffuse scattering from dislocation loops and solute precipitates, energy-resolved X-ray scattering, quasi-elastic scattering, phase transformations, theory of scattering of electrons and X-rays from defects in solids.

OAK RIDGE NATIONAL LABORATORY (continued)

237. RESEARCH USE OF THE LOW-TEMPERATURE IRRADIATION FACILITY

H. R. Kerchner, C. E. Klabunde
Phone: (615) 574-6270

$1,182,000 02-4

Operate for users a Low-Temperature Neutron Irradiation Facility (LTNIF) at ORNL Bulk Shielding Reactor. Determine neutronics characteristics in the irradiation cryostat for use at an in-core position and with several radiation modifying devices. Design and construct specialized cryogenic test equipment. Equipment and procedures for the transfer of irradiated specimens at 4.2 K. Development of a transmission electron microscopy facility for study of solids irradiated at low temperatures without warmup. Radiation effects in high T_c superconductors.

238. SURFACE PHYSICS AND CATALYSIS

D. M. Zehner, A. P Baddorf, H. L. Davis, G. R. Gruzalski, J. R. Noonan, J. F. Wendelken
Phone: (615) 574-6291

$886,000 02-5

Studies of crystallographic and electronic structure of clean and adsorbate-covered metallic and semiconductor surfaces, combined techniques of low-energy electron diffraction (LEED), photoelectron spectroscopy (PES) using synchrotron radiation, and computer simulations for surface crystallography studies with emphasis on surfaces which either reconstruct or have inter-planar spacings different from those of the bulk, LEED, PES, and Auger electron spectroscopy (AES) combined with in situ laser annealing of semi-conductors, lineshape analysis of Auger spectra, LEED, AES and X-ray photo-electron spectroscopy (XPS) studies of both clean and adsorbate-covered surfaces of metals, intermetallic compounds and carbides, determination of effects of intrinsic and extrinsic surface defects on surface properties using LEED, vibronic structure of adsorbates examined by high-resolution electron energy loss spectroscopy (EELS), examination of surface electronic and geometric structures with respect to solid state aspects of hetero-geneous catalysis.

OAK RIDGE NATIONAL LABORATORY (continued)

239. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND COLLABORATIVE RESEARCH CENTER

C. W. White, J. B. Roberto, O. E. Schow III, T. P. Sjoreen, S. P. Withrow
Phone: (615) 574-6295

$1,076,000 02-5

The SMAC Collaborative Research Center provides facilities for materials alteration and characterization in a UHV environment. Methods which can be used for alteration include ion implantation, ion beam mixing, and pulsed laser irradiation. In situ characterization methods include Rutherford backscattering, ion channeling, low-energy nuclear reaction analysis, and surface analysis techniques. The facility supports research in the Ion Beam Analysis and Ion Implantation Program and research carried out by other ORNL divisions. These facilities are available to scientists from industrial laboratories, universities, other national laboratories, and foreign institutions for collaborative research projects.

240. ION BEAM ANALYSIS AND ION IMPLANTATION

C. W. White, M. J. Aziz, J. H. Barrett, R. Feenstra, S. Gorbatkin, O. W. Holland, J. C. McCallum, C. J. McHargue, D. B. Poker, O. E. Schow, J. M. Williams, S. P. Withrow
Phone: (615) 574-6295

$1,100,000 02-5

Studies of ion implantation damage and annealing in a variety of crystalline materials (semiconductors, metals, superconductors, insulators, etc.), formation of buried amorphous or insulating layers by high dose ion implantation, formation of superconducting thin films by electron beam evaporation, fundamental studies of ion beam mixing in metal/semiconductor, metal/metal, and metal/insulator systems, applications of ion beam mixing and ion implantation to corrosion/catalysis studies, to reduction of friction and wear of metal surfaces, to changes in mechanical and optical properties of ceramics and insulators, to reduction of corrosive wear of surgical alloys, diffusion in amorphous semiconductors, pulsed-laser annealing and rapid solidification, high speed crystal growth phenomena, solute trapping and solute segregation at ultra rapid growth velocities, formation of supersaturated alloys, formation of epitaxial thin films by direct ion beam deposition, studies of ion channeling phenomena.

OAK RIDGE NATIONAL LABORATORY (continued)

241. ION BEAM DEPOSITION

R. A. Zuhr, T. E. Haynes, J. B. Roberto
Phone: (615) 576-6722

$405,000 02-5

Direct ion beam deposition of isotopically pure thin films on metal and semiconductor substrates using decelerated ion beams from an ion implantation accelerator, use of low-energy (10-200 eV) ion beams to alter surface atom mobilities and phase formation, fabrication of epitaxial layers and heterostructures by ion beam deposition at low temperatures, production of oxides and thin magnetic films, investigation of low-energy ion-solid interactions including ion beam etching and damage processes.

242. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION

W. S. Aaron, H. L. Adair, M. Petek, J. R. Gibson
Phone: (615) 574-5916

$345,000 02-5

Research and development of preparative techniques applicable to isotopic materials. Stable and radioactive isotopes are prepared in the form of ultra-thin films (supported and self-supported), coatings, wires, rods, cast shapes, alloys, compounds, ceramics, cermets, and distilled metals; techniques of preparation include vapor deposition, sputtering (rf, dc, planar magnetron, and ion beam), rolling, electrodeposition, molecular plating, liquid phase and conventional sintering, hot pressing, reduction/distillation, conversion of organic precursors to oxide films and solid forms, He implantation in metals, and general inorganic chemical processing. In-house characterization methods include X-ray diffraction and fluorescence, metallographic and ceramographic sample preparation, optical microscopy, scanning electron microscopy with energy dispersion X-ray spectrometry, differential thermal analysis, microgravimetric determinations, thermal conductivity determination, in situ film thickness monitoring, and sophisticated radiation counting methods.

OAK RIDGE NATIONAL LABORATORY (continued)

243. INVESTIGATIONS OF SUPERCONDUCTORS WITH HIGH CRITICAL TEMPERATURES

F. W. Young, Jr., L. A. Boatner, W. L. Bond, J. Brynstead, J. D. Budai, W. H. Butler, D. K. Christen, R. Feenstra, D. M. Kroeger, S. H. Liu, H. A. Mook, S. J. Pennycook, D. B. Poker, S. T. Sekula, B. C. Sales, E. Sonder, J. R. Thompson, J. Z. Tischler
Phone: (615) 574-5501

$500,000 02-5

Studies of a new class of perovskite-type oxides with high superconducting transition temperatures. Synthesis, characterization, and analysis, thin films and devices, and high current conductors. Magnetization measurements of $ReBa_2Cu_3O_7$ superconductors. Collaborative research with scientists at Lawrence Berkeley Laboratory and Los Alamos National Laboratory.

Materials Chemistry - 03 -

M. L. Poutsma - Phone (FTS) 624-5028 or (615) 574-5028

244. CHEMISTRY OF ADVANCED INORGANIC MATERIALS

E. J. Kelly, C. E. Bamberger, G. M. Begun, G(ilbert) M. Brown, J. Brynestad, L. Maya, C. E. Vallet
Phone: (FTS) 624-5024 or (615) 574-5024

$1,200,000 03-1

Application of ion implantation and ion beam mixing to the generation and systematic study of surface-modified materials of interest as catalysts, e.g., $M_xT_{1-x}O_2/Ti$ (M = Ru, Ir, Rh, etc.) for electrocatalysis of Cl_2 and O_2 evolution; determination of the mechanism of the catalyzed reaction, nature of the catalyst, and its specific mode of operation via electrochemical, Rutherford backscattering, and in situ photoacoustic and photocurrent spectroscopic techniques. Development of new generalized methodologies for the synthesis of nonoxidic ceramic materials (BN, Si_3N_4, SiC, C-B-N ternaries, and the borides, carbides, carbonitrides, and nitrides of the transition metals of groups 4, 5, and 6) in powder, fiber, film, or whisker forms; pyrolysis or photolysis of inorganic or organometallic precursors (e.g., synthesis of Ti, Zr, and Nb nitrides and carbonitrides via pyrolysis of the ammonolysis products of the transition metal halides or dialkylamides; synthesis of semiconducting C-N-B thin films via pyrolysis of borazine derivatives); synthesis of BN, SiC, and TiN (whiskers) via reactions of molten NaCN with BPO_4, SiO_2, and TiO_2, respectively. Synthesis and characterization of superconducting oxides.

OAK RIDGE NATIONAL LABORATORY (continued)

245. STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS

A. H. Narten, B. K. Annis, G(eorge) M. Brown, W. R. Busing,
D. W. Noid, B. Wunderlich
Phone: (FTS) 624-4974 or (615) 574-4974
$1,165,000 03-2

Characterization of polymers and composites at the molecular level by neutron and X-ray scattering studies and by thermal analysis; prediction of conformational, thermodynamic, and dynamics propertes through advanced computing and statistical mechanical techniques; relationship of structure to physical properties; development of synchrotron radiation scattering and neutron spectroscopic techniques. Materials studied include high-performance crystalline fibers and composites, conducting polymers and small-molecule models for polymers.

246. THERMODYNAMICS AND KINETICS OF ENERGY-RELATED MATERIALS

T. B. Lindemer, A. L. Sutton, Jr.
Phone: FTS 624-6850 or (615) 574-6850
$350,000 03-2

Determination and modeling of phase equilibria and other thermochemical data, as well as of reaction kinetics important to energy-related ceramic systems. Our new adaptations of chemical-mathematical models from the literature are used to represent the chemical thermodynamic interrelationship of temperature, oxygen chemical potential, and nonstoichiometry. These efforts provide a heretofore unavailable, generalized chemical thermodynamic description of nonstoichiometric oxide solutions. One current emphasis is the chemical thermodynamic description of the $YBa_2Cu_3O_{7-x}$ superconducting oxide, as well as of the Y-Ba-Cu-O system in general. A second emphasis is the experimental determination of the chemical kinetics of silicon nitride decomposition at 1500-2000 K in the presence of carbon under controlled chemical potentials of N_2, O_2, and/or H_2, particularly those typical for internal combustion engines.

OAK RIDGE NATIONAL LABORATORY (continued)

247. NUCLEATION, GROWTH, AND TRANSPORT PHENOMENA IN HOMOGENEOUS PRECIPITATION

C. H. Byers, M. T. Harris
Phone: (FTS) 624-4653 or (615) 574-4653

$320,000 03-2

Fundamental laser light-scattering spectroscopic studies and theoretical framework for liquid-phase homogeneous nucleation and growth of pure component and composite monodisperse metal oxide particles which are precursor materials in ultra fine processing for the production of a new generation of ceramic materials. Investigation of metal alkoxide/metal salt reactions and reactants-solvent interactions (i.e., short range bonding) which affect the characteristics of the particles formed. Determination of transport properties (i.e., viscosity and diffusivity) which provide important clues to the behavior of the fluid media in which particle growth occurs. Methods and instrument development (including alternative methods for metal oxide powder synthesis, optical spectroscopic measurements, low angle-light scattering spectrometer design, dispersion stabilization, and mathematical analysis).

248. ADVANCED NEUTRON SOURCE

C. D. West, G. L. Copeland, R. M. Harrington, R. E. Pawel, D. L. Selby, P. B. Thompson, M. K. Wilkinson
Phone: (615) 574-0370

$2,500,000 04-1

Preconstruction R&D associated with the Advanced Neutron Source (ANS) at ORNL. Core physics, neutronics, and thermal hydraulics for preconceptual core design. Construction and operation of corrosion and thermal-hydraulic test loop to study oxide formation and growth. U_3Si_2 fuel experiments and evaluations of new fuel plate designs. Preconceptual design of a cold source. Construction of cold source test facility. Safety investigations, risk analyses, project planning, and preliminary building design. Planning of facilities for neutron scattering, isotope production, and materials irradiation.

OAK RIDGE ASSOCIATED UNIVERSITIES
Oak Ridge, TN 37831

Metallurgy and Ceramics - 01 -

Keith Newport - Phone (FTS) 626-3422 or (615) 576-3422

255. OAK RIDGE SYNCHROTRON ORGANIZATION FOR ADVANCED RESEARCH

T. A. Habenschuss, C. J. Sparks, R. DeAngelis, S. Moss, R. Young
Phone: (615) 574-6996

$105,000 01-1

A synchrotron radiation beam line installed by the Oak Ridge National Laboratory at the National Synchrotron Light Source at Brookhaven is made available to interested users from university and industrial laboratories. University staff and industrial scientists are invited to join in collaborative research in materials science of importance to DOE programs at a large and unique research facility not available at their home institutions. More than twenty institutions are presently members. The beam line will supply focused X-radiation spanning the energy spectrum from 3 to 40 KeV at energy resolutions of delta $E/E = 2 \times 10^{-4}$. One Oak Ridge Associated University staff member is stationed at the NSLS to interface with the users and to develop computer programs for data acquisition and analysis. Among the research capabilities available on this beam line are: crystallography on small samples, structure of amorphous materials both liquid and solid, diffuse X-ray scattering from crystalline defects, short-range order and atomic displacements, and X-ray spectroscopy of electron rearrangements.

[redacted] SHARED RESEARCH EQUIPMENT PROGRAM (SHARE)

E. A. Kenik
Phone: (615) 574-5066

$100,000 01-1

Application of microanalysis facilities for collaborative research in materials science by members of universities or industry with ORNL staff members. Facilities include state-of-the-art analytical transmission electron microscopy, high voltage electron microscopy, field ion microscopy/atom probe surface analysis, and nuclear microanalysis instrumentation. Electron microscopy capabilities include analytical electron microscopy [energy dispersive X-ray spectroscopy (EDXS), electron energy loss spectroscopy (EELS) and convergent beam electron diffraction (CBED)], high voltage electron microscope in situ studies, and high resolution electron microscopy. Surface analysis facilities include four Auger electron spectroscopy (AES) systems and two Van de Graaff accelerators for Rutherford backscattering and nuclear reaction techniques.

PACIFIC NORTHWEST LABORATORY
P. O. Box 999
Richland, WA 99352

G. L. McVay, Materials Sciences Coordinator

Metallurgy and Ceramics - 01 -

G. L. McVay - Phone (FTS) 444-3762 or (509) 375-3762

260. MICROSTRUCTURAL MODIFICATION IN CERAMIC PROCESSING USING INORGANIC POLYMER DISPERSANTS

G. J. Exarhos, D. M. Friedrich (PNL); I. A. Aksay (University of Washington)
Phone: (509) 375-2440

$310,000 01-1

The goal of this program is to develop a fundamental understanding of structure-property relationships for inorganic polymers so that they can be tailored as dispersion agents for ceramic powder. The near-term goals are to investigate the structural effects on polymer-ceramic and polymer-solvent interactions. Alterations of inorganic polymers on ceramic surfaces as a function of temperature are also being investigated. Improvements in the consolidated ceramic mechanical properties are being measured as well as defect concentrations and distributions.

[redacted] FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

R. H. Jones, D. R. Baer, M. J. Danielson, M. A. Friesel
Phone: (509) 376-4276

$440,000 01-2

Investigations of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium nickel, and nickel-based alloys in gaseous and aqueous environments with and without gamma radiolysis. Relationships between grain boundary chemistry, hydrogen embrittlement, and intergranular stress corrosion cracking investigated with surface analytical tools, electrochemical polarization, straining electrode tests, subcritical crack growth tests, and crack-tip and fracture surface analysis. Modeling of the electrochemical conditions at the tip of a growing crack and evaluation of the electrochemical behavior of sulfur and phosphorus in the grain boundaries of nickel. Acoustic emission analysis of stress corrosion cracking processes. Effect of plastic strain and gaseous environments (O_2, H_2O, and H_2O+Cl) on adsorption processes studied with an in situ Auger electron spectroscopy straining stage.

PACIFIC NORTHWEST LABORATORY (continued)

262. LEACHING OF GLASS AND CERAMICS

L. R. Pederson, K. F. Ferris
Phone: (509) 375-2731

$370,000 01-3

Mechanistic studies of the interactions of silicate glasses and crystalline ceramics with aqueous environments, by systematic variation of bulk structure, surface properties, and solution chemistry. Structural studies consider the influence of bridging/nonbridging oxygen ratios, extent of polymerization, and redox effects on leachability. Surface electrical properties in solution, sorption phenomena, and the nature of an altered surface layer are included in studies of the effects of surface properties on leaching. Solution chemistry parameters of interest include pH, Eh, ionic strength, saturation with respect to key glass components, and the use of isotopically-labelled water.

263. IRRADIATION-ASSISTED STRESS CORROSION CRACKING

R. H. Jones, E. P. Simonen
Phone: (509) 376-4276

$200,000 01-4

The effects of radiation on material microstructure/microchemistry and water chemistry is being evaluated with respect to the mechanisms of stress corrosion in a radiation environment. Research includes radiation effects on segregation, sensitization, crack-tip phenomena, and water chemistry. The effect of radiation on crack-tip chemistry is being evaluated using a combination of crack-tip chemistry and radiolysis computer codes.

PACIFIC NORTHWEST LABORATORY (continued)

Solid State Physics - 02 -

G. L. McVay - Phone (FTS) 444-3762 or (509) 375-3762

264. THIN FILM OPTICAL MATERIALS

K. F. Ferris, G. J. Exarhos, D. M. Friedrich, C. B. Duke (Xerox Webster Research Center)
Phone: (509) 375-2440

$244,000 02-2

Theoretical and experimental study of basic physical properties that control the optical behavior of dielectric materials in thin-film form. Measure, model, and understand how the behavior of thin-film optical structures depends on materials properties. Materials studied include elemental semiconductors and their oxides and nitrides. Materials properties studied include composition, stoichiometry, phase structure, strain, and stress. Optical and material characterization techniques include Raman spectroscopy, X-ray diffraction, laser interferometry, total integrated and angular scattering, and resonant cavity reflectometry.

Materials Chemistry - 03 -

G. L. McVay - Phone (FTS) 444-3762 or (509) 375-3762

265. CERAMIC COMPOSITE SYNTHESIS UTILIZING BIOLOGICAL PROCESSES

P. C. Rieke, G. L. McVay (PNL); I. A. Aksay (University of Washington); A. H. Heuer, A. I. Caplan, (Case Western Reserve University)
Phone: (509) 375-2833

$250,000 03-1

Studies of natural formation of hard tissue that use polymers as templates to control and orient ceramic crystal growth. Crystal growth on modified polymer surfaces, particle growth in vesicles, and cell control of crystal growth. Surface, interface and colloid chemistry of small atom cluster. Modeling of polymer surfaces and interactions with ions in solution.

SANDIA NATIONAL LABORATORIES
P. O. Box 5800
Albuquerque, NM 87185

F. L. Vook, Materials Sciences Coordinator - Phone (FTS) 844-9304
or (505) 844-9304

Metallurgy and Ceramics - 01 -

R. E. Loehman (Acting) - Phone (FTS) 844-4069 or (505) 844-4069

275. PHYSICS AND CHEMISTRY OF CERAMICS

A. Hurd, B. C. Bunker, K. D. Keefer, D. W. Schaefer, C. J. Brinker,
B. D. Kay, C.H.F. Pedan
Phone: (505) 846-3551

$1,225,000 01-1

Multidisciplinary studies to relate molecular structure of ceramics to physical properties. The objective is to develop a fundamental understanding of the precursor prepration and consolidation processes required to produce novel and superior ceramics. Characterize sol-to-gel and gel-to-glass transitions in the silica system using SAXS, NMR, and light scattering to determine structures of the pre-gel phase, random colloidal aggregates, and the gel-to-glass conversion; model structure of porous materials using concepts of fractal geometry to predict structure from solution chemistry, and model sintering and absorption characteristics of random porous materials. Prepare ceramic superconductors and other electronic ceramics by novel solution processing.

S. T. Picraux - Phone (FTS) 844-7681 or (505) 844-7681

276. ION IMPLANTATION AND DEFECTS IN MATERIALS

S. T. Picraux, S. M. Myers, K. L. Brower, B. L. Doyle,
H. J. Stein, D. M. Follstaedt, J. A. Knapp, W. R. Wampler,
L. E. Pope, N. R. Sorensen, A. D. Romig, R. J. Bourcier
Phone: (505) 844-7681

$979,000 01-3

Ion implantation and ion beam mixing used with laser and electron-beam heating to form novel metastable and equilibrium microstructures in solids. Characterization of the evolution and final states of these systems by ion-beam analysis, TEM, EPR, optical absorption, X-ray scattering, AES, XPS, time-resolved reflectivity, time-resolved electrical conductivity, and mechanical and electrochemical testing. Utilization of such methods for fundamental studies of metastable amorphous and crystalline alloys, superlattices, defects in semiconductors, synthesis of novel layered structures, rapid-solidification processes in semiconductors and metals, properties of hydrogen in metals, diffusion in amorphous alloys, and mechanical and chemical effects of ion implantation. Investigation of consequences for semiconductor-device development, fusion energy, hydrogen storage, coatings technology and corrosion.

SANDIA NATIONAL LABORATORIES (continued)

F. L. Vook, Phone (FTS) 844-9304 or (505) 844-9304

277. ADVANCED GROWTH TECHNIQUES FOR IMPROVED SEMICONDUCTOR STRUCTURES

S. T. Picraux, A. W. Johnson, J. Y. Tsao, K. P. Killeen,
B. W. Dodson, I. J. Fritz, E. Chason, B. L. Doyle, K. Horn
Phone: (505) 844-7681
$381,000 01-3

Advanced growth techniques are studied for the synthesis of new and improved epitaxial semiconductor heterostructures. The primary growth techniques of molecular beam epitaxy (MBE) and metallorganic chemical vapor deposition (MOCVD) are used in conjunction with laser and ion beam stimulation to develop new crystal growth techniques. Initial studies concentrate on layered III-V compounds and Si/Ge strained layer structures, with emphasis on beam-enhanced techniques to allow a wider range of nonequilibrium growth conditions and thus to widen the window of compositions and combinations that can be grown. Advanced in situ electron and X-ray diffraction analysis yields surface-structure information for correlation with growth parameters. Theoretical studies using atomistic and continuum modeling address stability limits, beam depostion and beam-enhanced growth in conjunction with the above experimental studies.

P. S. Peercy, Phone (FTS) 844-4309 or (505) 844-4309

278. STRAINED-LAYER SUPERLATTICE MATERIALS SCIENCE

P. L. Gourley, R. M. Biefeld, L. R. Dawson, I. J. Fritz,
E. D. Jones, S. K. Lyo, G. C. Osbourn, J. Y. Tsao, B. W. Dodson
Phone: (505) 844-1556
$420,000 01-5

Study and application of compound semiconductor strained-layer superlattices and heterojunction quantum well materials to explore solutions to new and existing semiconductor materials problems. The program coordinaties semiconductor physics and materials science to produce new semiconductor materials with useful electronic properties not available in bulk compound semiconductor crystals. This program investigates fundamental material properties including band structure, electronic transport, crystal stability, optical transitions, and nonlinear optical properties. Both theoretical and experimental understanding are emphasized. The materials under study have a wide range of applications for high speed switching and microwave technologies, optical detectors, lasers, and optical modulation and switching.

SANDIA NATIONAL LABORATORIES (continued)

Solid State Physics - 02 -

G. A. Samara - Phone (FTS) 844-6653 or (505) 844-6653

279. TAILORED SURFACES FOR MATERIALS APPLICATIONS

J. E. Houston, G. L. Kellogg, R. R. Rye, J. W. Rogers, Jr., N. D. Shinn, P. J. Feibelman
Phone: (505) 844-6653

$633,000 02-2

The overall goal of this program is to develop an understanding of the fundamental nature of surface modification which will improve our ability to tailor the structure and electronic properties of surfaces and interfaces for specific materials applications. The research is focused on two important aspects of tailored surfaces and interfaces: (1) studies of the modification of surface structure and electronic properties by adsorbates and (2) studies of the interfaces that are developed when thin overlayers are deposited on single crystal surfaces. Fundamental understandings of surface and interfacial structure and bonding are critical to our ability to predict effects related to epitaxial growth, metallization, interface diffusion, and adhesion. These properties of the interface are becoming increasingly more important to the production and performance of microelectronic and other advanced microscale technologies where the "material" is effectively becoming a series of interfaces.

J. E. Schirber - Phone (FTS) 844-8134 or (505) 844-8134

280. PHYSICS AND CHEMISTRY OF NOVEL SUPERCONDUCTORS

D. S. Ginley, D. R. Jennison, J. F. Kwak, B. Morosin, J. E. Schirber, E. Stechel, E. L. Venturini
Phone: (505) 846-2529

$540,000 02-2

The fundamental physical properties of the copper oxide based high temperature superconductors. Directed toward understanding the detailed electronic band structure, doping, and carrier transport in these materials, especially as they pertain to understanding metal-insulator transitions, superconductivity, and the role of oxygen in determining transport properties. Unique and specialized instrumental capabilities including conductivity, photoconductivity, thermal conductivity, heat capacity, magnetotransport, de Haas van Alphen, thermopower and tunneling. Experiments at temperatures as low as 0.05 K, magnetic fields up to 120 kOe and hydrostatic pressure to 10 kbar in various combinations. An active in-house synthesis program, unique processing capabilities including high pressure, high temperature oxygen.

SANDIA NATIONAL LABORATORIES (continued)

J. E. Schirber - Phone (FTS) 844-8134 or (505) 844-8134

281. VERY HIGH TEMPERATURE SEMICONDUCTING BORIDES

D. Emin, T. L. Aselage, A. N. Campbell, B. Morosin, C. L.
J. Adkins, A. C. Switendick, D. R. Tallant, E. L. Venturini
Phone: (505) 844-3431
$500,000 02-5

Electronic, magnetic, optical, vibrational, and structural properties of very high temperature semiconducting borides. To understand fundamental properties of these materials sufficiently well for use as innovative electronic and optical semiconductor devices for use at exceptionally high temperatures. Materials synthesis with variety of techniques. Materials to be studies as to macro- and micro-structure with HRTEM, X-ray and neutron scattering, and Auger analysis. Very high temperature electronic transport studies (conductivity, Hall effect and Seebeck coefficient measurements) in collaboration with JPL. Pressure dependence of conductivity and Hall mobility to be studied. Magnetic susceptibility and ESR will be investigated. Thermal conductivity, specific heat, velocity of sound and thermal properties measurements.

Materials Chemistry - 03 -

J. B. Gerardo - Phone (FTS) 844-3871 or (505) 844-3871

282. CHEMICAL VAPOR DEPOSITION AND SURFACE PHOTOKINETIC RESEARCH

A. W. Johnson, W. G. Breiland, P. Ho, M. E. Coltrin,
J. R. Creighton, C. I. H. Ashby, M. E. Riley
Phone: (505) 844-8782
$457,000 03-3

Studies of important vapor-phase reactions and nucleation processes during CVD deposition under conditions used to fabricate photovoltaic cells, corrosion-resistant coatings, and semiconductor devices. Measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Test of our predictive model, which includes chemical and fluid dynamics. Study and development of laser CVD, laser photochemical deposition and etching, and laser-based fabrication of small-dimension structures. Application of our laser-based measurement capabilities to the study of vapor phase reactions of these laser processing techniques and application of surface measurement techniques to study the product materials. Fundamental study of the interactions of photons and molecules near and on surfaces. Auger, Sims, and laser-based measurements of surfaces in situ to deposition and etching. Development of model for combined laser, admolecule, and surface dynamics.

SANDIA NATIONAL LABORATORIES
Livermore, CA 94550

Metallurgy and Ceramics - 01 -

P. L. Mattern - Phone (FTS) 234-2520

[redacted]. FORMATION AND ANALYSIS OF HIGH-TEMPERATURE [redacted] AND THIN FILMS

M. Lapp, K. F. McCarty, J. C. Hamilton
Phone: (415) 294-2435 or FTS 234-2435
$295,000 01-1

Laser-based diagnostic studies of interfacial phenomena occurring during the growth and processing of thin films. Emphasis is on the phase composition and structure of thin films, and the study of solid-state reactions occurring between interfaces. Material systems studied include ceramic high temperature superconductors, multicomponent oxide films, thin-film protective coatings, and metal-dielectric interfaces. Formation techniques include high-temperature oxidation, reactive sputtering, plasma processing, and combustion deposition. In situ laser-based diagnostics are used to study film growth and post-growth processing, such as phase modifications in [redacted]s, and to characterize the evolution of [redacted] with changing conditions (e.g., temperature), in real time and with high temporal resolution. Raman scattering is used to determine phase composition, and nonlinear optical spectroscopies, primarily surface second harmonic generation, are utilized to determine the symmetry and electronic structure of extremely thin films and buried interfaces.

[redacted] GASES IN METALS/COMPUTATIONAL MATERIALS/VISITING SCIENTIST PROGRAM

M. I. Baskes, G. J. Thomas, M. S. Daw, S. M. Foiles, W. G. Wolfer, J. S. Nelson, S. Robinson, S. Goods, C. M. Rohlfing, M. Mills, T. Lowe, T. E. Felter
Phone: (FTS) 234-3226 or (415) 294-3226
$980,000 01-2

Investigations of the behavior of hydrogen, tritium and helium in metals involving joint theoretical and experimental research. Experimental techniques include mechanical property measurements, electron microscopy, positron annihilation, and small angle neutron scattering, applied to tritiated metals and also metals implanted with helium below the damage threshold. A new theoretical method (Embedded Atom Method) developed to calculate the cohesive energy of metals and alloys with chemically active impurities which is being used to investigate the atomistic processes of fracture, dislocation motion, and chemistry at surfaces and grain boundaries. Investigate equilibrium structure of alloys, such as Ni_3Al, both in the bulk and at interfaces including the effects of adsorbates and alloying additions. Joint collaboration on the theoretical aspects of this program with visitors to Sandia, Livermore.

SANDIA NATIONAL LABORATORIES - LIVERMORE (continued)

292. IN SITU DIAGNOSTICS FOR [redacted]S AND THIN FILMS

M. Lapp, R. J. Anderson, J. C. Hamilton
Phone: (415) 294-2435 or FTS 234-2435
$236,000 02-2

Develop and evaluate advanced, nonperturbing, interface-sensitive diagnostic techniques for materials research to produce data in real time and in situ. Focus on initial surface effects during exposures to reactive atmospheres, often at high temperature. Probe surface and near-surface layers with spontaneous Raman scattering, including the capability for Raman microprobe spectroscopy with a controlled-atmosphere environmental hot stage. Nonlinear optical spectroscopies, in particular second harmonic generation, are exploited to study surface processes at submonolayer coverages. The dynamics of surface reactions will be investigated using ultrafast spectroscopic techniques. Recent results include real-time studies of species and reactions at interfaces, with current efforts on hydrogen and carbon monoxide adsorption, [redacted], and carbon formation on metal crystals.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, CO 80401

D. Feucht - Phone (FTS) 327-7718 or (303) 231-7718

Solid State Research Branch - 02

S. Deb - Phone (FTS) 327-1105 or (303) 231-1105

296. SEMICONDUCTOR THEORY

A. Zunger
Phone: (303) 231-1172 or (FTS) 327-1172

$185,000 02-3

First-principles band structure, total energy, and statistical mechanical (cluster variation) methods are used to predict electronic and structural properties of ordered semiconductors and their alloys, emphasizing chemical trends and properties of new materials. Current work includes (1) first-principles prediction of alloy thermodynamic quantities (e.g., enthalpies of formation) and complete temperature-composition phase diagrams for bulk $A_xB_{1-x}C$ semiconductor alloys (e.g., $Ga_{1-x}In_xP$, including order/disorder transitions, miscibility gaps, and ordered stoichiometric compounds). These methods have also been applied to a metallic case, Cu_xAu_{1-x}; (2) novel ordering in ternary compounds [e.g., $(GaAs)_m$, $(GaSb)_n$ or HgTe/CdTe superlattices]; (3) calculation of valence band offsets between II-VI and III-V semiconductors; (4) prediction of properties of unusual ternary materials, e.g., ordered vacancy $A^{II}B_2^{III}C_4^{IV}$ compounds (e.g., $CdIn_2Se_4$), and filled tetrahedral compounds $A^IB^{II}C^V$ (e.g., LiZnAs); (5) calculations of <u>epitaxial</u> phase-diagrams intended to understand epitaxial stabilization, e.g., bulk-insoluble components becoming epitaxially soluble (GaP_xSb_{1-x}); appearance of epitaxial compounds with no bulk counterpart (SiGe) or epitaxial phase transitions (B1-like CdTe, B3-like MgS). Theoretical tools include (a) the total energy non-local pseudopotential method, (b) the all-electron Mixed Basis Potential Variation band structure method, (c) the total energy full-potential linearized augmented plane wave (LAPW) method, and (d) the cluster variation approach to the Ising problem, applied to binary or pseudobinary phase diagrams.

STANFORD SYNCHROTRON RADIATION LABORATORY
Stanford University
P. O. Box 4349, Bin 69
Stanford, CA 94309-0210

Solid State Physics - 02 -

A. I. Bienenstock - Phone (FTS) 462-3153 or (415) 926-3153

298. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES

A. I. Bienenstock, H. Winick
Phone: (415) 926-3153

$4,940,000 04-1

Support of materials research utilizing synchrotron radiation, as well as operations and development of the Stanford Synchrotron Radiation Laboratory (SSRL). Development and utilization of new methods for determining atomic arrangements in amorphous materials, static and time-resolved studies of highly perfect semiconductor crystals using X-ray topography, photoemission studies of semiconductor interfaces (e.g., heterojunctions and Schottky barriers), metal surfaces (especially catalytic reactions on surfaces) and development of techniques such as surface EXAFS, photoelectron diffraction, photon stimulated desorption and interface studies using core level spectroscopy.

Development of techniques for the non-invasive visualization of the human circulatory system, particularly of the coronary arteries. Development of techniques for inelastic X-ray scattering to measure the dynamic structure factor of condensed matter excitations, including phonons and electronic excitations. Development of ultra-high resolution scattering techniques, by means of resonant nuclear scattering.

SECTION B

Grant Research

(Primarily Universities)

The information in this Section was prepared by the DOE project monitors of the Division of Materials. There is considerable turnover in the Grant Research program, and some of the projects will not be continued beyond the current period.

ARIZONA STATE UNIVERSITY
Tempe, AZ 85287

[redacted] HIGH RESOLUTION ENERGY LOSS RESEARCH: Si COMPOUND CERAMICS AND COMPOSITES

R. W. Carpenter
Center for Solid State Science
Phone: (602) 965-4544
S. H. Lin
Dept. of Chemistry
Phone: (602) 965-3715

$124,999 01-1

High spatial resolution analytical electron investigation microscopy with a field emission source of the elemental composition and local electronic structure of small amorphous and crystalline regions in SiC and Si_3M_4 and in interfacial reaction zones of metal/ceramic and ceramic/ceramic composites. Development of theoretical methods for EELS spectral analysis. Quantitative analysis of small-probe current distribution in real and reciprocal space for field emission gun analytical electron microscopes to permit quantitative analysis of compositional gradients.

351. SURFACE STRUCTURES AND REACTIONS OF CERAMICS AND METALS

J. M. Cowley
Dept. of Physics
Phone: (602) 965-6459

$105,000 02-2

Studies of surface structures of small crystals of oxides and metals and of reaction of metals with oxides under the influence of intense ionizing radiation and heat using advanced electro-optical techniques; high resolution electron microscopy (HREM), microdiffraction, and electron energy loss spectroscopy (EELS). Measurements in ultra-high vacuum environment in which the specimen may be prepared and treated. The metal oxide specimens include samples with particle diameter of <1 nm, important for catalytic systems and thin surface layers significant for bonding. Investigation of effects of ionizing radiation and the presence of surface layers of water, oxygen, or other gases. Excited states of small particles and the modification of the energetics as a function of particle environment are also studied.

UNIVERSITY OF ARIZONA
Tucson, AZ 85721

[redacted]. [redacted]

P. A. Deymier
Department of Materials Science and Engineering
Phone: (602) 621-6080

$147,640 01-1

Study of properties of [redacted] in pure metallic and alloy systems. Experiments coupled with dynamical atomistic computer simulations. Measurement and calculation of excess free energy of anisotropic interfaces. Description of the grain boundary phase equilibrium diagram. Study of phase transitions of grain boundaries. Examination of solute atom segregation at boundaries in alloys and effect on interfacial properties. Mg, Al, and Mg-Al alloys.

353. ARTIFICIALLY LAYERED SUPERCONDUCTORS

C. M. Falco
Dept. of Physics
Phone: (602) 621-6771

$110,505 02-2

Investigation of the nature of artificial metallic multilayer systems, their electronic and superconducting properties including Josephson junction and weak link characteristics. Fabrication of superlattices with greater perfection and understanding of the important fabrication parameters. Preparation of layered materials both with a three-gun magnetron sputtering system and by molecular epitaxy. Use of X-ray diffraction, resistance, Rutherford backscattering (RBS), TEM, Mossbauer spectroscopy, electron tunneling, High - and Low-Energy Electron Diffraction (HEED and LEED) to characterize samples. Emphasis is on the superconducting properties of the superlattice systems to develop materials, weak links and microbridges with improved operating characteristics.

ATLANTA UNIVERSITY
Atlanta, GA 30314-4381

354. CERAMIC MATERIALS FROM PRECERAMIC ORGANOMETALLIC COPOLYMERS

Y. H. Mariam
Dept. of Chemistry
Phone: (404) 653-8593

$ 73,920 01-3

Preparation of ceramics via polymer chemistry. Chemical manipulation of derived copolymers with reactive functional groups leads to in-situ bulk state cross-linking and metal incorporation process operations. Curing, thermolysis and pyrolysis reactions monitored using IR, ESCA, and cross polarization/magic angle spinning NMR techniques to analyze composition, structure and elemental constitution along the reaction path. Correlation of chemical intermediate characteristics with ceramic microstructural, chemical and mechanical properties.

BOEING AEROSPACE COMPANY
Seattle, WA 98124

355. X-RAY SPECTROSCOPIC INVESTIGATION OF RADIATION DAMAGED MATERIALS

R. B. Greegor
Phone: (206) 655-0514
F. W. Lytle
Phone: (206) 655-5574

$ 86,747 01-1

EXAFS/XANES techniques are used to determine the structural arrangements in minerals naturally occurring in a metamict state: titanates, zircons, thorites, monazites, huttonites, fergusonites, and perovskites. Comparison is made to the synthetic mineral actinide-doped (e.g., Pu in thorite, $ThSiO_4$) or ion-implanted, or otherwise radiation damaged. Assessment is made of the long term stability of titanate, phosphate and silicate radioactive wasteforms which would be subject to the same processes of radiation damage and geochemical alteration in waste containment applications as metamict minerals.

BOSTON UNIVERSITY
Boston, MA 02215

356. THE GEOMETRY OF DISORDER: THEORETICAL INVESTIGATIONS OF QUASICRYSTALS AND FRUSTRATED MAGNETS

C. H. Henley
Physics Department
Phone: (617) 353-2600

$ 73,509 02-3

Develop complete atomic structural models for quasicrystals and systematically fit them to available diffraction data (in collaboration with AT&T Bell Labs) for the two known structural types, Al-Mn and Al-Zn-Mg, using appropriate geometric framework and atom decoration. Develop quantitative predictions for low-temperature specific heat, tunneling dynamics and spin-wave excitations in spin glass models. Study diluted frustrated system relations to spin glasses for uniformly frustrated vector-spin systems and continue efforts to understand low-temperature, slow dynamics due to barrier activation of spin systems at percolation.

357. ATOMIC BEAM STUDIES OF THE INTERACTION OF HYDROGEN WITH TRANSITION METAL SURFACES

M. M. El-Batanouny
Dept. of Physics
Phone: (617) 353-4721

$110,000 02-4

Use of inelastic surface scattering of neutral atomic and molecular beams to investigate (1) the different mechanisms for hydrogen exchange between particular crystal faces and the bulk and the relationship between these mechanisms and the rate of hydrogen uptake into the bulk in niobium, palladium, and tantalum, (2) energy exchange on transition metal crystal faces between rotational and translational excitations, (3) hydrogen-induced surface structural changes on Pd(110) and Fe(110), (4) lattice dynamical calculations to enhance the understanding of the experimental observations. A study of surface magnetism on iron and copper crystals using spin polarized metastable behavior scattering.

BRANDEIS UNIVERSITY
415 South Street
Waltham, MA 02254

358. SYNTHESIS AND PROPERTIES OF NOVEL, ELECTROACTIVE ORGANOMETALLIC POLYMERS

M. Rosenblum
Dept. of Chemistry
Phone: (617) 647-2807

$ 75,000 03-1

Synthesis of organometallic polymers based on transition metal complexation of rigidly held aromatic five and six membered rings. The aromatic ring will be held in a framework such that electron or hole conduction should occur through overlap of the pi-orbitals on contiguous facing aromatic rings. The C_6-based polymers will be derived from paracyclophenes and the C_5 polymers from cyclopentadienylnaphthalene.

BRIGHAM YOUNG UNIVERSITY
Provo, UT 84602

[redacted] INFLUENCE OF [redacted] DISTRIBUTION AND PROCESSING HISTORY IN INTERGRANULAR CREEP CAVITATION

B. L. Adams
Dept. of Mechanical Engineering
Phone: (801) 378-3843

$ 54,833 01-2

Studies of intergranular creep cavitation in alloy 304 stainless steel as a function of a) grain boundary misorientation angle, b) grain boundary surface orientation, and c) multiaxial stress state. SEM and TEM diffraction characterizations of boundary structure and cavitation damage. Processing effects on grain boundary structure distribution and damage susceptibility.

BROWN UNIVERSITY
Providence, RI 02912

360. FATIGUE CRACK GROWTH UNDER FAR-FIELD CYCLIC COMPRESSION

S. Suresh
Div. of Engineering
Phone: (401) 863-2626

$119,913 01-2

Experimental and theoretical investigation of crack growth under far-field cyclic compression at both ambient and elevated temperatures in single phase ceramics, transformation-toughened ceramics (partially-stabilized zirconia), a ceramic-matrix composite and model metallic systems. A detailed investigation of the compression fatigue behavior at elevated temperatures, representative of potential in-service applications, is planned. Secondarily, investigate the feasibility of controlled crack growth in compression fatigue as a pre-cracking technique for the fracture testing of a variety of ceramic materials. Program will lead toward a fundamental understanding of the mechanics and mechanisms of fatigue crack growth at ambient and elevated temperatures from which guidelines for fatigue design involving advanced engineering materials will evolve.

361. SURFACES AND THIN FILMS STUDIED BY PICOSECOND ULTRASONICS

H. J. Maris
Dept. of Physics
Phone: (401) 863-2185
J. Tauc
Dept. of Physics
Phone: (401) 863-2318

$152,400 02-2

Thin films, interfaces, coatings and other surface layers investigated using very high frequency (10 - 500 GHz) sound. The ultrasound will be produced by light pulses with duration of less than one picosecond. Fundamental studies of lattice dynamics and the propagation of sound under conditions of high damping. The method will be developed into a nondestructive testing technique of the mechanical properties of films and interfaces and the detection of structural flaws with significantly better resolution than presently available.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA 91125

362. THE KINETICS OF SHORT RANGE ORDERING IN UNDERCOOLED ALLOYS

B. T. Fultz
Dept. of Materials Sciences
Phone: (818) 356-2170

$107,614 01-1

Study of kinetics of short range order in undercooled alloys of Fe-Al, Fe-Si, and Fe-Co having highly disordered states. Ordering at low temperatures characterized by Mossbauer and EXAFS spectrometries. Comparison of experimental results with Monte Carlo computer simulations of short range order kinetics. Study of short range order in alloys with dilute ternary additions to determine effects of ternary solutes on kinetics and thermodynamics of ordering.

[redacted] STUDIES OF ALLOY STRUCTURE AND PROPERTIES

W. L. Johnson
Dept. of Engineering and Applied Science
Phone: (818) 356-4433

$295,935 01-1

Synthesis, structure, and properties of amorphous alloys, the principal aim of which is to understand the thermodynamics and kinetics of phase transformations in and the structure of noncrystalline materials. Characterization of the electronic structure of metallic glasses and its relation to atomic structure; and investigations of the formation of glassy materials prepared by solid state reactions, ion-beam mixing, and rapid quenching. Atomic structure studies include use of EXAFS, XANES, SAXS, SANS, Mossbauer spectroscopy, and NMR. Electronic structure is probed by measuring specific heats, transport properties, and superconductivity.

CALIFORNIA INSTITUTE OF TECHNOLOGY (continued)

364. MELTING IN ADSORBED FILMS

D. L. Goodstein
Dept. of Physics, Mathematics, and Astronomy
Phone: (818) 356-4319

$112,000 02-2

This program involves thermodynamic and pulsed NMR studies of adsorbed films. Heat capacity and vapor pressure measurements are being made on a systematic grid of points in the coverage versus temperature plane. A detailed phase diagram for methane adsorbed on graphite has been developed from the thermodynamic data. The combination of thermodynamic and NMR data is being used to investigate the nature of melting at the crossover between 2 and 3 dimensions.

CALIFORNIA STATE UNIVERSITY/FULLERTON
Fullerton, CA 92634

[redacted] QUANTITATIVE SYNCHROTRON TOPOGRAPHY: ASSESSMENT AND CONTROL OF LOCAL STRAIN FIELDS IN HIGH TEMPERATURE AND ADVANCED ELECTRONIC MATERIALS

J. C. Bilello
School of Engineering and Computer Science
Phone: (714) 773-3362

$120,000 01-1

Real-time quantitative methods of X-ray topography as a non-destructive tool to study the mechanical stability of surfaces and interfaces. Research focused on: (a) interaction of plastic deformation with grain boundaries in a high-temperature refractory metal (Mo) and (b) studies of high-performance coatings of refractory metals (W, Nb, and Mo) on single-crystal substrates (Si). Synchrotron X-ray topography studies at SSRL and NSLS.

UNIVERSITY OF CALIFORNIA/DAVIS
Davis, CA 95616

366. INVESTIGATION OF THE RATE-CONTROLLING MECHANISM(S) FOR HIGH TEMPERATURE CREEP AND THE RELATIONSHIP BETWEEN CREEP AND MELTING BY USE OF HIGH PRESSURE AS A VARIABLE

H. W. Green
Dept. of Geology
Phone: (916) 752-1863
A. K. Mukherjee
Dept. of Mechanical Engineering
Phone: (916) 752-1776

$141,531 01-2

Determine the pressure dependence of high-temperature creep of nickel, cesium chloride, silicon and forsterite. Study activation volume and its relationship to partial molar volume of diffusing species. Provide data for critical tests of creep theories.

367. CHEMICAL DECOMPOSITION OF CERAMICS UNDER IRRADIATION

D. G. Howitt
Dept. of Mechanical Engineering
Phone: (916) 752-0580

$115,000 01-4

Investigation of electron and ion irradiation induced ionization, displacement damage, diffusion, and stimulated desorption by means of in situ electron microscopy and mass spectroscopy. Study of ion mixing effects under ion irradiation. Finite difference solutions to a two dimensional diffusion equation for the irradiation and desorption process. Materials: Na-αAl_2O_3, Na borosilicate glass, TiC.

368. AN INVESTIGATION OF THE MECHANISMS OF SOLID STATE POWDER REACTIONS IN THE COMBUSTION SYNTHESIS AND SINTERING OF HIGH TEMPERATURE MATERIALS

Z. A. Munir
Dept. of Mechanical Engineering
Phone: (916) 752-0559

$ 87,000 01-5

Reaction mechanisms in powder synthesis with emphasis on the process of combustion synthesis and the concomitant sintering. Low-temperature diffusional processes and their effect on the combustion process. Powder interactions and their effect on the sintering of the product phase. Combustion wave velocities and activation energies. Effects of powder particle size and distribution, surface layers and contamination, and thermal history. Materials investigated: Al and Ni alloys, silicides.

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, CA 92717

369. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

J. C. Hemminger
Dept. of Chemistry
Phone: (714) 856-6020

$170,000 02-2

Investigation, by means of Raman scattering spectroscopy, of the molecular adsorbates on well characterized metal surfaces to further elucidate the origin of the surface enhanced scattering, and in conjunction with other surface science probes to study surface chemistry. Determination of the active form of corrosive agents. Bonding of corrosive inhibitors to metal surfaces. Correlation of Raman enhancement with the electronic energy levels of the metal-adsorbate system that will be determined with high resolution electron energy loss spectroscopy and photoemission. Use of ultra-high-vacuum surface apparatus with computer controlled Raman scattering spectrometer.

370. INELASTIC ELECTRON SCATTERING FROM SURFACES

D. L. Mills
Dept. of Physics
Phone: (714) 856-5148

$136,040 02-3

Theory of the inelastic scattering of electrons, ions, and neutral atoms from elementary excitations at surfaces, and the development of theoretical descriptions of these excitations. Emphasis on electron energy loss from surface phonons at both clean and adsorbate-covered surfaces. Studies of spin-slip scattering of low energy electrons from magnetic excitations at surfaces, and excitation of surface phonons by helium atoms. Strong emphasis on the quantitative comparison between the results of this program and experimental data. Tightly coupled effort between Professor Mills and Professor Tong at the University of Wisconsin at Milwaukee.

UNIVERSITY OF CALIFORNIA/LOS ANGELES
Los Angeles, CA 90024

371. AMORPHIZATION OF METALLIC ALLOYS UNDER PROTON AND NEUTRON IRRADIATION

A. J. Ardell
Dept. of Materials Science and Engineering
Phone: (213) 825-7011
C. N. J. Wagner
Dept. of Materials Science and Engineering
Phone: (213) 825-6265

$108,583 01-4

Investigation of the crystalline to amorphous transformation in proton irradiated intermetallic compounds. Effects of dose, temperature, and irradiating particle. Transformation monitored by TEM, X-ray diffraction, and DSC.

372. QUANTUM FLUCTUATIONS IN MESOSCOPIC SYSTEMS

SheChao Feng
Dept. of Physics
Phone: (213) 825-8530

$ 50,500 02-2

The electronic properties, especially conductance properties, of very small (10-100 A) metallic and semiconducting structures will be studied theoretically. Several effects must be considered together, including quantum coherent effects on the transport, and multiple scattering due to disorder in the conductor. Similar theoretical approaches will be applied to describe the magnetic properties of spin glasses. The dynamical properties of percolating systems, in particular the low-energy excitations of tenuous, "fractal", systems, will be investigated.

373. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

G. A. Williams
Dept. of Physics
Phone: (213) 825-8536

$180,000 02-5

Investigation of the nonlinear nonequilibrium properties of materials including quantum fluids. Localization of vibrational energy in condensed matter, especially in discreet classical models consisting of chains of simple coupled nonlinear vibrators. Acoustic models of nonlinear systems such as high amplitude vibrations of flat plates and cylindrical shells. Nonlinear dynamical effects in convecting dilute solutions of ^3He in superfluid ^4He including mode locking between two intrinsic oscillatory modes, and investigation of generalized scaling laws. Quantum fluids including the nucleation of the A --> B transition of ^3He and spin-polarized hydrogen isotopes.

UNIVERSITY OF CALIFORNIA/SAN DIEGO
La Jolla, CA 92037

374. INVESTIGATION OF SUPERCONDUCTIVITY AND MAGNETISM IN d- AND f-ELECTRICAL MATERIALS

M. B. Maple
Dept. of Physics
Phone: (619) 534-3330

$350,000 02-2

Investigations on a variety of rare earth and actinide compounds, including studies of superconductivity, magnetism, and effects that arise from their mutual interaction, as well as the anomalous behavior exhibited by heavy electron (or "heavy Fermion") materials that is associated with valence fluctuations and the Kondo effect. Measurements of ac and dc magnetic susceptibility, specific heat, and electrical resistivity under conditions of temperature between 80 milliKelvin and 300 K, magnetic fields to 10 Tesla, and pressures to 160 kbar.

375. PREPARATION AND CHARACTERIZATION OF SUPERLATTICES

I. K. Schuller
Dept. of Physics
Phone: (619) 534-2540

$153,103 02-2

Preparation and characterization of superlattices with constituents that do not form solid solutions in their binary phase diagrams. Search for new superlattices; study relationship between epitaxial and superlattice growth; compare samples prepared by sputtering and thermal evaporation. Use of molecular beam epitaxy (MBE), sputtering. Growth studies with Nb/Cu. Roughness measurements with Ge/Pb multilayers. Characterization of samples by X-ray diffraction, electron microscopy, and in situ high energy electron diffraction. Measurement of other properties, i.e., transport, magnetic, optical, superconducting, etc., in collaboration with others.

[redacted] ION MIXING AND SURFACE MODIFICATION IN METAL SEMICONDUCTOR SYSTEMS

S. S. Lau
Dept. of Electrical Engineering and Computer Sciences
Phone: (619) 534-3097
J. Mayer
Dept. of Materials Science and Engineering (Cornell University)
Phone: (607) 255-7273

$144,000 (30 months) 02-4

Experimental investigation of the ion mixing during and following ion implantation. Metal-semiconductor bilayer samples. Nickel-silicon system with silicide formation. Germanium-silicon alloys in contact with near noble metals. Ion mixing and thermal annealing process comparison.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, CA 93106

[redacted] STRUCTURE AND CHEMISTRY OF METAL/CERAMIC INTERFACES

M. Rühle
Materials Department
Phone: (805) 961-8275

$120,000 01-1

Different metals and ceramics joined under well-defined, instrumented, bonding conditions. Reaction layers for different metal/ceramic combinations identified and quantified by analytical electron microscopy. Defect structure determined by high resolution electron microscopy. Theoretical models of bonding and chemistry of interfaces developed.

378. CONDENSED MATTER RESEARCH USING THE UCSB FREE ELECTRON LASER

V. Jaccarino
Dept. of Physics
Phone: (805) 961-2121
L. Elias
Dept. of Physics
Phone: (805) 961-4387

$ 87,100 02-2

Condensed matter research using a far-infrared free electron laser. Shallow impurity states in semiconductors. Cyclotron resonance in n-GaAs. Nonlinear excitation of lower dimensional electron systems. FIR-visible double resonance. Nonlinear excitation of magnons of arbitrary k. Suhl instability in antiferromagnetic FeF_2. Generation of high frequency phonons. Dynamics of impurity associated local modes. Phonon detection by coherence loss.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

[redacted] RESEARCH IN THEORIES OF PATTERN FORMATION AND NONEQUILIBRIUM PROCESSES

J. S. Langer
Dept. of Physics
Phone: (805) 961-3247

$136,352 02-3

Theoretical studies of pattern-forming processes primarily of importance to the solidification of metallurgical and other technological materials. Specific studies of boundary-layer models of dendritic solidification and generalization of these to realistic models, including effects of impurities and of "noisy" perturbations. Theory of pattern selection in directional solidification in alloys, of precipitation kinetics and statistical theory of the kinetics of phase separation. Development of new theoretical techniques, and investigation of their applicability to other phenomena, e.g. in fracture mechanics, in biological materials.

380. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino
Physics Dept.
Phone: (805) 961-2871
J. R. Schrieffer
Physics Dept.
Phone: (805) 961-2800
R. L. Sugar
Physics Dept.
Phone: (805) 961-3469

$134,323 02-3

Development of stochastic numerical techniques for simulating many-body systems containing particles that obey Fermi statistics, and application of these techniques to problems of strongly interacting fermions. One-dimensional and quasi-one-dimensional systems, arrays of these and extensions to higher dimensions. Investigations with various electron-phonon interactions to further the fundamental understanding of conducting polymers, spin glasses, and pseudo-random spin systems such as CeNiF. Non-phonon pairing models (e.g., excitonic, localized spin fluctuations). Consideration of correlation effects and frequency dependent transport to test the validity of theoretical approximations. Investigations of many-fermion systems in two and higher dimensions.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

381. MOLECULAR PROPERTIES OF THIN ORGANIC INTERFACIAL FILMS

J. Israelachvili
Dept. of Chemical and Nuclear Engineering
Phone: (805) 961-2902

$170,265 03-1

Fundamental measurements of structural, adhesive and tribological properties of thin organic films on solid surfaces. Film deposition by Langmuir-Blodgett method. Measurements emphasize the use of a Surface Forces Apparatus (SFA) for measuring directly the forces acting between solid surfaces as a function of separation with a distance resolution of 0.1 nm. Adhesion and surface energy of metals coated with surfactant and polymer films are measured by SFA in both gaseous and liquid environments. New measurements of dynamic forces acting on two laterally moving surfaces, recording the normal (compressive) and tangential (frictional) forces while simultaneously monitoring the plastic deformation.

382. POLYMERS AT SURFACES

P. A. Pincus
College of Engineering
Phone: (805) 961-4685

$105,000 03-2

Theoretical research on the interaction of polymers with surfaces. Effects of long rearrangement times leading to quasi-irreversibility and hysteresis in the force between polymer clad surfaces. Polymer absorbed on fluid-fluid interfaces. Dispersion stability of suspended colloids with absorbed polymers. Interaction of charged polymers with surfaces. Effects of adsorbed polymer layers on the spectrum and damping of capillary waves at the fluid-fluid interface.

UNIVERSITY OF CALIFORNIA/SANTA CRUZ
Santa Cruz, CA 95064

383. EXPERIMENTAL STUDIES OF CRITICAL BEHAVIOR IN SYSTEMS WITH QUENCHED DISORDER

D. Belanger
Dept. of Physics
Phone: (408) 429-2871

$108,000 02-1

Understand phase transitions and critical phenomena in systems with random, quenched disorder. Dilute cubic systems under uniaxial pressure and magnetic fields. Compare with random anisotropy and q=3 random field Potts models. Techniques of quasielastic and Bragg neutron scattering, spin echo neutron scattering, and optical linear birefringence. Improve high magnetic field and low temperature capabilities of birefringence equipment. Prepare and characterize samples including epitaxial thin films.

UNIVERSITY OF SOUTHERN CALIFORNIA
Los Angeles, CA 90089

384. DEFORMATION TWINNING IN ORDERED ALLOYS

E. Goo
Dept. of Materials Science
Phone: (213) 743-0961

$ 87,080 01-2

Determination of twinning mechanisms in ordered cubic alloys by use of high resolution electron microscopy. Investigation of effect of degree of order, as determined by X-ray diffraction techniques, on twin formation. Materials with three different structures to be studied are TiNiFe, Ni_3Al and CuZnAl.

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

385. THE EFFECTS OF APPLIED STRESS ON MICROSTRUCTURAL EVOLUTION

W. C. Johnson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-8785
D. E. Laughlin
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2706

$112,404 01-1

Theoretical and experimental study of second phase morphology changes in alloys due to the influence of an applied stress field. Morphological characteristics include precipitate shape, size and distribution. Theoretical studies to identify the relative effects of elastic misfit, elastic inhomogeneity, precipitate interaction and the nature of the applied stress field on precipitate size and the evolution of precipitate shape. Computer simulations of the effect of the elastic interaction of precipitates on coarsening under applied stress fields. Experimental studies on Ni-Al and Ni-Al-X two-phase alloys of the effects of stress on microstructure to compare to theoretical predictions and to document effects of precipitate interactions on precipitate shape.

386. PHASE SEPARATION AND ORDERING IN InGaAsP AND InGaAs MATERIALS

S. Mahajan
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2702
D. E. Laughlin
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2706

$195,000 01-1

Experimental study (X-ray diffraction and transmission electron microscopy) of phase separation, ordering and coarsening in InGaAs and InGaAsP grown by liquid phase epitaxy and given thermal treatments. Evaluation of electrical mobilities (using the technique of vander Pauw) and optical properties (assessed by photoluminescence). Studies of the influence of microstructural features on dislocation grids (with and without optical pumping) for correlation with degradation resistance of InP/(In,Ga)(As,P) and GaAs/(Ga,Al)As light emitting devices.

CARNEGIE MELLON UNIVERSITY (continued)

387. EQUILIBRIUM COMPOSITION OF INTERPHASE BOUNDARIES

P. Wynblatt
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-8711

$130,178 01-1

Combined experimental and theoretical study of solid interphase boundary composition. Experimental work to be carried out on interfaces produced via epitaxial films of Ag-Cu alloys doped with Au deposited on single-crystal sodium chloride; (001), (011), and (111) interface orientations of the Ag-rich and Cu-rich phases to be produced. Compositional data to be obtained from scanning Auger microprobe measurements using crater-edge profiling. Modeling to be carried out using the Embedded Atom Method with Monte Carlo techniques.

388. THE ROLE OF PASSIVE SURFACE FILMS ON CORROSION FATIGUE CRACK INITIATION

I. M. Bernstein
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2700
A. W. Thompson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2700

$187,577 (18 months) 01-2

Experimentally measure and model the roles of a passive surface layer and the underlying microstructure in controlling corrosion fatigue crack initiation and subsequent lifetimes. Investigate titanium containing varying amounts of solute oxygen in which key parameters can be controlled and independently measured in order to advance both the model and the general understanding of corrosion fatigue initiation under passive conditions. Develop a predictive electromechanical test to assess a particular alloy's susceptibility to corrosion fatigue.

CASE WESTERN RESERVE UNIVERSITY
Cleveland, OH 44106

389. MICROSTRUCTURE-MECHANICAL PROPERTY RELATIONSHIPS IN TRANSFORMATION-TOUGHENED CERAMICS

A. H. Heuer
Dept. of Metallurgy and Materials Science
Phone: (216) 368-3868

$ 56,325 01-2

Ostwald ripening in ZrO_2 toughened Al_2O_3. Plastic deformation in two-phase "single crystal" Ca partially-stabilized ZrO_2, and in 100 percent tetragonal ZrO_2 polycrystals. Stress-induced transformation in Y-TZP and ZTA. The focus of these studies is the nature and extent of the transformation zone associated with propagating cracks and the critical factors involved in processing strong and tough polycrystalline tetragonal ZrO_2. Correlation of TEM analysis with mechanical properties.

UNIVERSITY OF CHICAGO
Chicago, IL 60637

390. HIGH-TEMPERATURE THERMOCHEMISTRY OF TRANSITION METAL BORIDES AND SILICIDES

O. J. Kleppa
The James Franck Institute
Phone: (312) 702-7198

$ 66,596 01-3

Thermochemical investigation of transition metal borides and silicides of 4d and 5d transition metals by means of high temperature mixing calorimetry. Chart quantitatively systematic trends in the enthalpies of formation of congruent melting borides and silicides of the same stoichiometry. Obtain quantitative information relating to the dependence of the enthalpy of formation on the stoichiometry of the compound for selected binary systems.

UNIVERSITY OF CHICAGO (continued)

391. RESEARCH IN TWO DIMENSIONAL CRITICAL PHENOMENA AND CONFORMAL FIELD THEORY

D. Friedan
Enrico Fermi Institute
Phone: (312) 702-7119
S. Shenker
Enrico Fermi Institute
Phone: (312) 702-7187

$150,000 02-3

Research is conducted on a variety of topics in the theory of two-dimensional critical phenomena. Arithmetic conformal field theory. Two dimensional conformal field theory as modular geometry. A two-dimensional representation of the modular group on the four punctured sphere. Reconstruction of the puncture moduli space geometry from the fundamental modular geometry on the space of closed surfaces. Description of statistical mechanical systems as non-unitary (c=0) conformal field theories. Supersymmetry and the tricritcal Ising phase diagram. Supersymmetry and the 1-D quantum spin chain. Use of algebras of chiral quantum fields in conformal field theory.

UNIVERSITY OF CINCINNATI
Cincinnati, OH 45221

392. SURFACE CHEMISTRY OF ELECTROCATALYSIS

A. Hubbard
Dept. of Chemistry
Phone: (513) 475-2263

$112,955 03-2

Determination of the structure, composition, and electrochemical reactivity of electrocatalyst surfaces after various stages of pretreatment and use in solutions of hydrocarbons. Surface characterized by low-energy electron diffraction, compositions by Auger spectroscopy, thermal properties by thermal desorption mass spectroscopy, vibrational spectra by Fourier transform infrared spectroscopy, electron energy loss vibrational spectroscopy, and electrochemical behavior by potentiostatic voltametry. Objectives include comparison of the adsorption strengths of hydrocarbons such as hydroquinone and ethylene, solvents such as dimethyl sulfoxide, promoters such as iodide, and poisons such as carbon monoxide and aminoethanethiol on surfaces of copper, gold, platinum, and alloys of these elements.

CLARK COLLEGE
Atlanta, GA 30314

393. INVESTIGATIONS OF POLING PROCESSES, CHARGE TRAPPING AND PRESERVATION IN SOME FERROELECTRIC AND POLYMERIC MATERIALS

O. P. Puri
Division of Natural Sciences and Mathematics
Phone: (404) 681-3080, x200

$ 96,900 01-3

Investigation of the mechanism of formation and relaxation of electrets in nonpolar inorganic single crystals, polycrystalline and amorphous dielectrics. Experimental characterization of electret formation as a function of sample temperature polarization field, cooling rate, and electret decay in the open and closed circuit condition. Extension of Swann-Gubkin theory by considering the nonpolar part of electret polarization through ion displacement. Charge transport, space charge and defect diagnoses on oxides, chalcogenide glass and elemental Si samples.

COLORADO SCHOOL OF MINES
Golden, CO 80401

394. THE ROLE OF COMPOSITION AND MICROSTRUCTURE GRADIENTS ON WELD METAL PROPERTIES AND BEHAVIOR

D. L. Olson
Center for Welding Research
Phone: (303) 273-3787
D. K. Matlock
Center for Welding Research
Phone: (303) 273-3775

$175,023 01-5

The effects of weld metal compositional and microstructural gradients on phase transformations, microstructural stability, and mechanical properties considered on a fundamental basis in weld metal alloys that are primarily austenitic (e.g., stainless steels). Models, which incorporate compositional gradients, developed to predict the resulting weld metal properties. The mechanical properties of weld metals modeled based on composite theory in which individual weld metal zones are considered as discrete elements within a composite structure.

COLORADO SCHOOL OF MINES (continued)

395. FUNDAMENTAL OPTICAL STUDIES OF COMPETITIVE ADSORPTION AND THIN FILM PHENOMENA

T. E. Furtak
Dept. of Physics
Phone: (303) 273-3843

$109,000 02-2

Development of techniques for study of electrochemical environment, electrolyte-solid surface interface. In situ optical experiments. Dynamics and structure of the prototypical electrolyte-solid system. Interpretations from ab initio theories of metal surfaces, competitive adsorption, and liquid state. New instrumentation - second harmonic generation spectroscopy with a tunable laser source to identify surface nonlinear effects and relate to recent theories of second harmonic generation in thin films. Variation of incident photon energy is essential to probe the relative cross section of the electronic excitations.

COLORADO STATE UNIVERSITY
Fort Collins, CO 80523

396. PROPERTIES OF MOLECULAR SOLIDS AND FLUIDS AT HIGH PRESSURE AND TEMPERATURE

R. D. Etters
Dept. of Physics
Phone: (303) 491-5374

$ 71,000 02-3

Theoretical calculation of the properties of molecular solids and fluids over broad ranges of high temperatures and pressures. Properties of interest are as follows. Solids: equilibrium structures and orientations, lattice vibrational and vibrational mode frequencies, intramolecular vibron frequencies, sound velocities, equations of state, compressibilities, and structural and orientational phase transitions. Fluid phase: equations of state, vibron frequencies, the melting transition, specific heats, compressibilities, second virial coefficients, viscosities and other transport properties, and the nature of orientational and magnetic correlations. Techniques used include multi-dimensional optimization strategies, self-consistent lattice dynamics, constant pressure and constant volume Monte Carlo (i.e.,variable metric) computation, mean field and classical perturbation methods. Systems studied include N_2, O_2, CO, CO_2, F_2, N_2O, benzene, nitromethane, HCl, HBr, and H_2. Attention is given to connections to combustion and detonation phenomena, and to synthesis of new materials. Collaboration with theoretical work and close correlation with experimental programs at LANL.

UNIVERSITY OF COLORADO
Boulder, CO 80309

397. STUDIES OF MELTING, CRYSTALLIZATION, AND COMMENSURATE-INCOMMENSURATE TRANSITIONS IN TWO DIMENSIONS

W. J. O'Sullivan
Dept. of Physics
Phone: (303) 492-7547
R. C. Mockler
Dept. of Physics
Phone: (303) 492-8511

$126,840 02-2

Preparation and study of systems of synthetic colloidal microspheres that exhibit the primary phenomena of physical interest in lower dimensional systems. Use of e-beam lithography and film deposition to construct substrate particle-traps in extended or local patterns, to provide potential fields acting on the colloidal particles. Quasi-elastic light scattering microscopy combined with digital image processing, and various other optical techniques, applied to study colloidal particles in suspension films, monolayers, and bilipid membranes. Melting, crystallization, solid-solid transitions, fractal scale invariant coagulation, response of monolayer crystals to the equivalent of ultra high pressures, experimental and computer simulation of particle distributions and dynamics --including collapse of distributions on quenching electrostatic interparticle forces, critical diffusion rates in thin binary liquid films.

COLUMBIA UNIVERSITY
New York, NY 10027

398. PROTONS AND LATTICE DEFECTS IN PEROVSKITE-RELATED OXIDES

A. S. Nowick
Henry Krumb School of Mines
Phone: (212) 280-2921

$165,000 01-3

Defect chemistry of pure and doped $KTaO_3$ crystals, $LiNbO_3$ crystals, and $BaCeO_3$. Role of protons and nonstoichiometry in perovskite-related superconductors. Dielectric relaxation studies by both ac bridge, ionic thermocurrent, and thermally stimulated depolarization methods. EPR studies on crystals doped with Fe^{3+}, Cu^{2+}, Ni^{3+}, Co^{2+}, or Mn^{2+}. Carrier analysis by thermoelectric power measurements. Conductivity measurements as a function of temperature and controlled environment. ac complex impedance analysis. Monitoring of proton content in water vapor treated samples by observation of the intensity of infrared absorption due to OH stretching. Behavior and defect chemistry of hydrogen containing single crystal $LiNbO_3$ and polycrystalline $BaCeO_3$. Characterization of the effect of equilibration of a superconducting oxide with known partial pressures of oxygen and hydrogen.

UNIVERSITY OF CONNECTICUT
Storrs, CT 06268

399. A COHERENT MODEL OF MARTENSITIC NUCLEATION AND GROWTH

P. C. Clapp
Dept. of Metallurgy
Phone: (203) 486-4714

$105,719 01-1

Development of a model of coherent martensitic nucleation for a variety of transformation symmetries using a non-linear, non-local strain free energy similar to the Ginzburg-Landau form. Fourth-order gradient terms are included to deal with the large number of real systems showing negative second-order strain-gradient coefficients; heterogeneous defects of varying potencies are included; the dynamics of the transformation instabilities are analyzed for specific cases. One-, two-, and three-dimensional cases are studied and matched with the parameters of real systems. Point, line, and surface defects are considered and their effects, both local and global, on the transformation are examined. The model contains a self-consistency check on the coherency hypothesis; cases that fail this test are considered separately as this indicates an essential role for interface dislocations in the nucleation process.

400. FATIGUE OF FERRITIC AND AUSTENITIC STEELS AT ELEVATED TEMPERATURES

A. J. McEvily
Metallurgy Dept.
Phone: (203) 486-2941

$ 76,160 01-2

Studies of the load interaction effects in the near threshold region of ferritic steels. Study of the behavior of austenitic stainless steels at elevated temperatures in order to understand the nature of creep fatigue interaction in an alloy system prone to cavitation, a tendency absent in the ferritic steels.

UNIVERSITY OF CONNECTICUT (continued)

401. ENERGY TRANSFER & NONLINEAR OPTICAL PROPERTIES AT NEAR ULTRAVIOLET WAVELENGTHS: RARE EARTH 4F->5D TRANSITIONS IN CRYSTALS & GLASSES

D. S. Hamilton
Dept. of Physics and Institute of Materials Science
Phone: (203) 486-3856
R. H. Bartram
Dept. of Physics and Institute of Materials Science
Phone: (203) 486-4915

$ 86,339 02-2

Investigation of optical properties of rare earth ions, substitutionally doped into host crystals and glasses. Epecially near ultraviolet transitions, 4f to 5d, of these ions. Non-radiative relaxation processes, two step photoionization, and laser-induced diffraction gratings and phase conjugate wave generation.

CORNELL UNIVERSITY
Ithaca, NY 14853

402. THE MIGRATION OF [redacted] IN CERAMIC MATERIALS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

C. B. Carter
Dept. of Materials Science and Engineering
Phone: (607) 255-4797

$ 45,000 (6 months) 01-1

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic-covalent solids. Concerns include (1) misorientation between grains and boundary plane orientation, (2) geometry of interfacial dislocations and steps, (3) interfacial chemistry including local segregation and nonstoichiometry, and (4) interfacial pinning by pores or crystalline or amorphous pockets or films of a second phase. Materials include Al_2O_3, ZnO, Mg-Al spinel, Si, and Ge. Studies on both powder compacts and bicrystals involve visible light microscopy, electron microprobe analysis, and strong- and weak-beam, lattice fringe, X-ray energy dispersive and electron energy loss TEM analysis. Bicrystals of controlled orientation produced by hot pressing.

CORNELL UNIVERSITY (continued)

403. STRONG FIBERS

H. H. Johnson
Dept. of Materials Science and Engineering
Phone: (607) 255-2323

$175,000 01-1

Use of microfabrication technology to produce fibers of metals, ceramics and ductile intermetallic compounds. Deposition processes such as coevaporation, reactive evaporation, sputtering, ion beam mixing, etc., will be integrated with pattern generation by optical lithography to produce fibers with transverse dimensions in the micrometer range, and lengths from a few millimeters to several centimeters. Rutherford backscattering spectroscopy, X-ray diffraction, transmission electron microscopy and electron diffraction to characterize fiber composition and structure. Correlations between structure and deposition techniques and parameters, and also post deposition heat treatments. Crystalline, amorphous and nanoscale structures will be produced and characterized. Room and elevated temperature mechanical property characterization. Mixed oxide ceramic fibers and fibers of ductile intermetallic alloys.

404. FOCAL PROBLEMS IN MODULATED AND MARTENSITIC STRUCTURAL PHASE TRANSFORMATIONS IN ALLOYS AND PEROVSKITES

J. A. Krumhansl
Dept. of Physics
Phone: (607) 255-5261

$136,022 01-1

New theoretical approach to a microscopic description of martensitic transformation of the twinning type, based on nonlinear, nonlocal elastic displacement fields. Results applicable to both alloy martensitic transformations and high-Tc superconducting perovskites. Primary emphasis placed on microscopic models of phonon anomalies, nonlinear Ginzburg - Landau model free energies for structural studies, diffuse scattering, precursors and diffraction analysis, weakly first-order transformations and pseudo-critical behavior, and anomalous behavior in structural transitions.

CORNELL UNIVERSITY (continued)

405. STUDIES OF THE III-V COMPOUNDS IN THE MEGABAR REGIME

A. L. Ruoff
Dept. of Materials Science and Engineering
Phone: (607) 255-4161

$175,000 01-1

Crystal structure changes in III-V compounds as a function of pressure to 200-300 GPa (2-3 Mbar) with emphasis on the transformation from four-fold to six-fold coordination and on identifying the various phases present with six-, eight-, and twelve-fold coordination. Acquisition of data over a broad range of pressure, coordination number, and interatomic spacing to test and promote the development of theoretical models. Development of energy dispersive X-ray analytical techniques in conjunction with a wiggler at the CHESS facility to obtain diffraction patterns to 100 keV. Development of diamond anvil cell techniques to 300 MPa and improved monochromatic powder diffraction.

406. EXPERIMENTAL STUDIES OF THE [redacted]

S. L. Sass
Dept. of Materials Sciences and Engineering
Phone: (607) 255-5239

$210,000 01-1

Investigation of grain boundary structure of BCC metals, ceramics, and intermetallic compounds using transmission electron microscopy and electron diffraction, and X-ray diffraction techniques, study of the influence of segregation on the structure of grain boundaries in Fe-base alloys, MgO + Fe and Ni_3Al, studies of grain boundary region in order to obtain structural information.

CORNELL UNIVERSITY (continued)

407. UHV-STEM STUDIES OF NUCLEATION AND GROWTH OF THIN METAL AND SILICIDE FILMS ON SILICON

J. Silcox
School of Applied and Engineering Physics
Phone: (607) 255-3332
E. J. Kirkland
School of Applied and Engineering Physics
Phone: (607) 255-3332

$175,000 01-1

Investigation of initial stages of thin film formation on silicon by UHV STEM techniques to determine the changes in atomic, chemical and electronic structure as compound formation proceeds. Initial systems chosen for study are the heavy transition metals, platinum, tungsten, and gold on silicon (111). Establishment of single atom visibility (and resolution) using annular dark field techniques and a new UHV method of preparation of single crystal, defect-free thin films of silicon. Computer based image simulation and enhancement techniques, together with electron microdiffraction. Experimental studies of films within the same microscope chamber will include AES, EELS, and XMPA spectroscopy to monitor chemical and electronic structure.

[redacted] AN INVESTIGATION OF MECHANICAL BEHAVIOR OF POLYCRYSTALLINE SOLIDS

C-Y. Li
Dept. of Materials Science and Engineering
Phone: (607) 255-4349

$100,000 01-2

State-variable description of creep deformation and related phenomena in polycrystalline intermetallic alloys. Load relaxation experiments used over a wide range of strain rates. Mechanism of grain boundary sliding is emphasized. Approaches to be developed to improve the creep strength of intermetallic alloys.

[redacted] [redacted]IN DEFORMATION PROCESSING OF CERAMICS

R. Raj
Dept. of Materials Science and Engineering
Phone: (607) 255-4040

$182,500 01-2

Investigation of interfacial interactions occurring when alumina, zirconia and their mixtures are processed at temperatures sufficient to admit superplastic behavior. In-house-processed materials monitored for structural changes at [redacted] over appropriate stoichiometric and applied stress intervals. Theoretical modeling of chemical diffusion and deformation processes using acquired experimental data.

CORNELL UNIVERSITY (continued)

[redacted] DEFECT STUDIES IN III-V THIN FILM SEMICONDUCTORS

D. G. Ast
Dept. of Materials Science and Engineering
Phone: (607) 255-4140

$118,967 01-3

Study the correlation between the electronic properties, atomic structure, and local chemistry of defects in GaAs, GaAs-based ternaries and at the interface between GaAs, GaAs-based ternaries and Si. The main objectives of the proposed research: Clarify the core structure of clean and decorated defects. Investigate relation between decoration state and electrical activity using a combination of TEM, in situ EBIC, CL, PL, and DLTS. Particular emphasis is placed on interface dislocations in multilayer structures. Investigate changes in the electrical activity and structure of defects as a function of annealing conditions using capped anneals, non-capped anneals (vacuum), annealing with InGaAs J. Woodall method), and annealing under very slow CVD growth conditions. Investigate the structure of grain boundaries, with particular attention to the possible dissociation of asymmetric grain boundaries into subsets of symmetric boundaries. Study the electrical activity of such boundaries and the correlation with structure, especially symmetry. Identify annealing treatments which minimize the electrical activity of boundaries. Investigate the electrical activity of anti-phase boundaries in GaAs on Si and Ge as a function of their structure. Investigate the origin of CL contrast of Si-GaAs and its connection to the spatial variation of deep states, using a combination of EBIC, CL, TEM, and spatially resolved PL.

411. SURFACE PHASES AND THEIR INFLUENCE ON METAL-OXIDE INTERFACES

J. M. Blakely
Dept. of Materials Science and Engineering
Phone: (607) 255-5149

$144,763 01-3

Determination of phase diagrams for binary 2-dimensional adsorbed systems, such as S + O, on transition metals and effect of adsorbed phases on growth and morphological stability of oxide layers on these materials. Determination of long range order and transitions in the adsorbate phases by LEED and surface X-ray diffraction. Composition and bonding information from Auger and photoemission spectroscopy. Spectroscopic ellipsometry for oxide thickness determination and scanning tunneling microscopy for the study of surface phase morphology, interphase boundaries, and heterogeneous oxide-adsorbate surfaces.

CORNELL UNIVERSITY (continued)

412. DEFECTS AND TRANSPORT IN MIXED OXIDES

R. Dieckmann
Dept. of Materials Science and Engineering
Phone: (607) 255-4315

$128,020 01-3

Measurements of nonstoichiometry, electrical conductivity and cation tracer diffusivity in NaCl- and spinel-structured quaternary oxides containing transition metal cations. Data to be combined with theoretical studies and computer simulation in order to develop a model for point defect equilibria and related transport properties.

413. STRONGLY INTERACTING FERMION SYSTEMS: EMPHASES ON HEAVY FERMIONS

J. W. Wilkins
Dept. of Physics
Phone: (607) 255-5193

$ 72,000 02-3

Theory of heavy fermion behavior in lanthanide and actinide compounds, and more generally of systems with f and/or d electrons that are strongly interacting or correlated. Aims at understanding the occurrence or absence of heavy fermions in such systems, the nature of the low temperature coherent state and the transition to a Kondo-like state at higher temperatures, and an account of the unusual magnetic and superconducting properties of heavy fermion materials. Both the one and two impurity Anderson models are studied, the former within the framework of the self-consistent large N expansion approach, and the latter using a numerical renormalization group approach. A new study of high-Tc materials has begun with an emphasis on understanding the ground state of the two-dimensional Hubbard model and the effects of Coulomb correlations on the electronic band structure.

414. SYNTHESIS AND PROPERTIES OF NOVEL CLUSTER PHASES

F. J. Di Salvo
Dept. of Chemistry
Phone: (607) 255-7238

$169,000 03-1

Synthesis of new cluster compounds containing Nb, Ta, or Mo. Included are reactions with solvated halide clusters of both M_6X_8 and M_6X_{12} types concentrating on Nb_6I_{11} and solid state synthesis reactions at temperatures above 800°C. Study of Mo_3X_3 infinite chain clusters and polymer blends of these inorganic polymers with organic polymers. Synthesis of complexes of Nb_6I_8 with bifunctional ligands or with square planar metal organic or coordination complexes. Characterization by X-ray diffraction, Faraday balance for magnetic measurements, four probe resistance for conductivity, Hall effect, and magneto-resistance measurements.

DARTMOUTH COLLEGE
Hanover, NH 03755

415. [redacted] IN B2 ORDERED ALLOYS

I. Baker
Thayer School of Engineering
Phone: (603) 646-2184

$126,035 01-2

A study of the structure and properties of grain boundaries of the B2 ordered alloys FeAl and NiAl. Grain size and composition variations; compression and tension testing at room temperature. Grain boundary structure and chemistry determined by transmission electron microscopy and atom probe field ion microscopy; in-situ straining during microscopy to determine dislocation/bonding interactions; grain boundary structure determined by X-ray diffractometry and selected area channeling patterns. Geometric modeling of grain boundaries in B2 structures correlated with experimental results.

416. [redacted]D TOUGHNESS OF $L1_2$ INTERMEDIATE COMPOUNDS

E. M. Schulson
Thayer School of Engineering
Phone: (603) 646-2888

$129,871 01-2

Examine dislocation pileup/grain boundary accommodation model in more detail; carry out systematic in situ TEM deformation studies on Ni-rich, stoichiometric and Ni-lean Ni_3Al both with (0.35at%) and without boron; investigate grain boundary sliding in Ni_3Al by systematic experiments on the effects of grain size on high-temperature deformation (800-1200K) of Ni_3Al with (0.35at%) and without boron; investigate grain size effects on the strength and ductility of Ni_3Si by systematic experiments on the effects of grain size on the mechanical properties and resultant deformation structure; improve the toughness of Ni_3Al through grain shape control, i.e., generate equiaxed fine grain structure with simultaneous increase of aspect ratio; comparative tests (fibrous <u>vs</u>. equiaxed microstructures) performed at RT using Charpy impact technique. Subsequent fracture toughness measurements using standard ASTM procedures.

DARTMOUTH COLLEGE (continued)

417. EXCITONS IN SEMICONDUCTOR SUPERLATTICES, QUANTUM WELLS, AND TERNARY ALLOYS

M. D. Sturge
Dept. of Physics
Phone: (603) 646-2528

$269,500 (24 months) 02-2

Improve the understanding of optically excited states of "quantum well" and "superlattice" structures in which semiconductors with quite different band gaps are interleaved. Time-resolved tunable laser spectroscopy will be used to study phenomena such as: (1) The effect of atomic disorder on exciton dynamics. (2) The nature of excitons and their phonon interactions in short period superlattices (SPS), both strained and unstrained. (3) The exciton-exciton interaction. When the excitons are indirect, both in real and momentum space, (as in GaAs/AlAs SPS), this interaction may lead to a new type of electron-hole liquid. (4) Exciton-exciton interactions in superlattices. (5) New materials for quantum wells and superlattices.

UNIVERSITY OF DELAWARE
Newark, DE 19716

418. NEUTRON STUDIES OF LIQUID AND SOLID HELIUM

H. R. Glyde
Dept. of Physics
Phone: (302) 451-2661

$ 80,000 02-1

Theoretical calculations of properties of liquid and solid helium for direct comparison with neutron measurements. The aim is to interpret neutron scattering data, to investigate implications of experiments in terms of extant and new models, and to propose new experiments. Specific examples are: direct calculation of the dynamic form factor S(Q,w) in liquid ^{3}He for comparison with existing data to test models of the effective interactions between atoms in the liquid, calculations of the momentum distribution in liquid ^{3}He and in solid ^{4}He for comparison with experiments at IPNS(ANL), and to test the impulse approximation using models appropriate to solid ^{4}He. Development of a microscopic theory of liquid ^{3}He based on Green's function methods. Study of the dynamics and phase transitions in adsorbed rare gas monolayers, particularly for the light rare gases exhibiting prominent quantum effects which cannot yet be treated by molecular dynamics.

UNIVERSITY OF DENVER
Denver, CO 80208

419. RESIDUAL STRESSES AND THERMAL EXPANSION IN FIBER REINFORCED CERAMIC COMPOSITES

P. K. Predecki
Dept. of Engineering
Phone: (303) 871-2102

$ 68,000 01-2

Investigation of residual stresses and strains in ceramic fiber/ceramic matrix composites by X-ray diffraction to obtain the near surface stresses and neutron diffraction to obtain the bulk microstresses in each crystalline phase. Diffraction measurements as a function of temperature on well-characterized specimens in which either the thermal expansion of the matrix or the fiber surface treatment varied. Materials investigated include Al_2O_3 fibers in silicate glasses and glass ceramics, and SiC whiskers in Al_2O_3. Noyan-Cohen analysis accounting for 3-dimensional nature of stresses and including, where possible, separation of macrostresses and microstress components in each phase. Results correlated with mechanical properties and thermal expansion via existing models for composite behavior. The objective is to provide a test for such models and to see if the techniques used are useful for predicting the strength, toughness, and thermal expansion of these materials.

420. INVESTIGATE FRACTURE TOUGHNESS AND FRACTURE MECHANISMS USING ACOUSTIC EMISSION MEASUREMENTS

S. H. Carpenter
Dept. of Physics
Phone: (303) 871-2176

$83,330 01-5

Investigation to determine if meaningful correlations exist between fracture toughness and measurable acoustic emission parameters and to determine if specific fracture mechanisms can be identified and characterized by the acoustic emission they produce. A study, using premium grade 4340 steel, is intended to establish the detectability limit of acoustic emission measurements with regard to ductile tearing/microvoid coalescence. The correlation of acoustic emission and fracture toughness will be studied when the mechanisms of fracture toughness and fracture are altered by changes in the microstructure of Ti-6Al-4V. A systematic investigation will be made of the acoustic emission from spherical second phase particles in aluminum-silicon alloys.

DUKE UNIVERSITY
Durham, NC 27706

421. VISUALIZATION OF CONVECTION IN ^{3}HE-SUPERFLUID-^{4}HE MIXTURES

R. P. Behringer
Department of Physics
Phone: (919) 684-8140

$ 20,000 02-3

The flow patterns in ^{3}He-superfluid ^{4}He mixtures will be imaged and recorded by means of a special neutron camera and associated electronics. The preferential segregation of the highly-absorbing ^{3}He isotope to the superfluid vortices is what permits the imaging. Information will be obtained on wave number selection, pattern formation, and the onset of chaotic flow. In addition to the studies of convection, heat flow patterns at temperatures near the superfluid-normal transition will be studied.

FLORIDA STATE UNIVERSITY
Tallahasee, FL 32306

422. HE-ATOM SCATTERING APPARATUS FOR STUDIES OF CRYSTALLINE SURFACE DYNAMICS

J. G. Skofronik
Dept. of Physics
Phone: (904) 644-5497
S. A. Safron
Dept. of Chemistry
Phone: (904) 644-5239

$130,000 02-4

Construction of a He atom-surface scattering instrument and the study of the dynamics of crystalline surfaces by low energy He-atom scattering. Extraction from surface phonon data of information on the interactions between surface species and hence on their physical and chemical properties. Surface phonon dispersion curves obtained by time-of-flight methods from inelastic single atom-surface encounters. Corrugation of and energy levels in the He-surface potential, obtained from elastic specular and diffractive scattering. Information on relaxation phenomena obtained from measurements of phonon lifetimes. Studies envisaged include: (110) surfaces of Au, Pt, and Ir, which reconstruct as a function of temperature. Surfaces of layered dichalcogenide compounds (e.g., $TaSe_2$, $NbSe_2$), which exhibit a variety of transitions with decreasing temperature--including charge density wave formation.

UNIVERSITY OF FLORIDA
Gainesville, FL 32611

423. THE COUPLING OF THERMOCHEMISTRY AND PHASE DIAGRAMS FOR GROUP III-V SEMICONDUCTOR SYSTEMS

T. J. Anderson
Dept. of Chemical Engineering
Phone: (904) 392-2591

$84,158 01-3

Solid state galvanic cell measurements and high temperature micro-calorimeter measurements to determine thermodynamic properties of $Al_xGa_{1-x}Sb$ and $Al_xIn_{1-x}Sb$ alloys. Liquid phase component activities measured to determine the appropriateness of several solution models. The ternary Al-Ga-Sb phase diagram will be computed and compared to experimental data. The Al-In-Sb and Al-Ga-In-Sb phase diagrams will be predicted. Defect structure of the material will be investigated.

[redacted] MODERATE AND LOW TEMPERATURE OXIDATION OF CLEAN NICKEL, CHROMIUM, AND Ni-Cr ALLOYS

P. H. Holloway
Dept. of Materials Science and Engineering
Phone: (904) 392-6664
C. D. Batich
Dept. of Materials Science and Engineering
Phone: (904) 392-6630

$ 54,038 01-3

Investigation of low to moderate temperature (100K < T < 500K) oxidation of pure nickel, chromium and nickel-chromium alloy surfaces using Auger electron spectroscopy, angle-resolved X-ray photoelectron spectroscopy and ion scattering spectroscopy. Specific aspects of the oxidation to be studied include initial oxide nucleation, lateral oxide growth to form a coalesced layer, dissolution of the oxygen into the bulk and the effect of the initial oxide microstructure on the multilayer growth at high temperature.

UNIVERSITY OF FLORIDA (continued)

425. WETTING AND DISPERSION IN CERAMIC/POLYMER MELT INJECTION MOLDING SYSTEMS

M. D. Sacks
Dept. of Materials Science and Engineering
Phone: (904) 392-6676

$50,525 01-3

Wetting and dispersion behavior in ceramic/polymer melt injection molding systems. Contact angle measurements by the sessile drop method of polymer melts on bulk silica substrates and on model powder compacts formed with monosized, spherical particles of silica. Investigation of a range of wetting conditions by varying substrate (bulk powder compact) surface chemistry (e.g., surface hydroxylation), altering polymer chemistry (e.g., ethylene:vinyl acetate ratio in EVA copolymers), and coating agents. Relationship of wetting behavior to the state of dispersion in powder/polymer mixes prepared with monosized, spherical particles. Rheological characterization of the state of dispersion and relationships to injection molding behavior. Particle coagulation, steric stabilization, and dispersion stability phenomena. XPS, FTIR, and photon correlation spectroscopies and ellipsometry.

426. X-RAY SCATTERING STUDIES OF NON-EQUILIBRIUM ORDERING PROCESSES

S. E. Nagler
Dept. of Physics
Phone: (904) 392-8842

$ 80,000 02-2

A study of the kinetics of first order phase transitions in thin films of alloys using time resolved X-ray scattering to follow the development of order in films quenched from high temperatures. Effects of dimensionality on the kinetics and role of topological defects in the growth of ordered domains in the thin film samples.

427. STUDIES OF HEAVY FERMION SYSTEMS

G. R. Stewart
Dept. of Physics
Phone: (904) 392-9263

$ 80,000 02-2

Experimental investigations of "heavy fermion" system such as UBe_{13} and UPt_3 (irradiated), mainly through low temperature calorimetry, but also with electrical resistivity and magnetic susceptibility techniques. The goals of this research: examination of the interactions between f-electron sites and comparison with theoretical models proposed to explain the highly correlated high effective mass observed in heavy fermion systems; observation of the interplay between superconductivity, magnetism, and non-ordered behavior.

UNIVERSITY OF FLORIDA (continued)

428. SYNTHESIS OF MODEL POLYMERS AND RELATED STRUCTURES IN SUPPORT OF VINYL MONOMER GRAFTING STUDIES

T. E. Hogen-Esch
Dept. of Chemistry
Phone: (904) 392-2011
G. B. Butler
Dept. of Chemistry
Phone: (904) 392-2012

$ 99,560 03-1

Synthesis of graft copolymers based on polysaccharides and plysaccharide derivatives and synthesis of model polymers including water-soluble block copyolymers, star polymers, and cyclic polymers. Grafting by redox initiation, thermal decomposition, or nucleophilic displacement. Characterization by IR, NMR, size exclusion chromatography, viscometry, and osmometry. Studies of structure-rheology relationships.

GENERAL ELECTRIC RESEARCH AND DEVELOPMENT
Schenectacy, NY 12301

[redacted]. DEFORMATION AND DEFECTS IN LAVES-PHASE INTERMETALLIC COMPOUNDS

J. D. Livingston
Materials Laboratory, Alloy Properties Branch
Phone: (518) 387-6465

$101,676 01-2

Explore the microscopic mechanical behavior of the largest class of intermediate phases--Laves phases. To develop understanding of the strength, toughness, and ductility of representative Laves phases, and, by extension, other intermetallic compounds with complex crystal structures. Measurements of mechanical properties are coupled with TEM studies of defects in deformed samples and detailed consideration of dislocation energies and mobilities. Deformation and fracture modes studied by SEM to characterize fracture modes, markings around hardness impressions at various temperatures examined for evidence of slip, twinning, and fracture.

GEORGIA TECH RESEARCH CORPORATION
Atlanta, GA 30332-3368

430. A STUDY OF MECHANISMS OF TIME-DEPENDENT CRACK GROWTH AT ELEVATED TEMPERATURES

A. Saxena
Fracture and Fatigue Research Laboratory
Phone: (404) 894-2888

$127,723 01-2

Creep and creep-fatigue crack growth experiments at elevated temperature; characterization of the crack tip damage mechanisms including cavity sizes and distribution by use of techniques such as TEM, SANS, X-ray and electron radiography; characterization of the influence of loading transients.

431. CRYSTALLINE METAL-SEMICONDUCTOR SUPERLATTICES

A. Erbil
School of Physics
Phone: (404) 894-5207

$ 92,000 02-2

Emphasis on the growth of naturally layered oxide materials involving Y, Ba, and Cu. Unusual elemental stoichiometries have given indications of superconductivity above 500K. The processing conditions and the physical and electronic properties of the resulting materials will be studied systematically. Additional superconductivity studies will be conducted on copper-free layered materials based on Ti, Bi, and/or V.

Work will continue on the metallorganic chemical vapor desposition (MOCVD) of La, TaTe, PbTe, and CdTe superlattices. The thin films will be characterized for their structural, chemical, optical, and electrical properties. Special emphasis will be given to the search for high temperature superconductivity in the superlattices.

432. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDY OF THE GEOMETRY OF SURFACE CLUSTERS

U. Landman
School of Physics
Phone: (404) 894-3368

$194,750 02-3

Theoretical investigation of the fundamental processes that determine the structure, transformations, growth, electronic properties, and reactivity of materials and material surfaces. Analytical methods and molecular dynamics simulation development and application to phase transformations, solidification, and chemical reactivity with emphasis on systems relevant to energy technologies.

GEORGIA TECH RESEARCH CORPORATION (continued)

433. GROWTH, STRUCTURE AND STABILITY OF EPITAXIAL OVERLAYERS

A. Zangwill
Dept. of Physics
Phone: (404) 894-7333

$ 84,582 02-3

Investigate growth, structure and stability of epitaxial overlayers. Morphology of MBE and CVD films by use of continuum models. Long-term evolution of morphological instability. Epitaxial stabilization of metastable phases. Development of a general theory of structural phases and phase transitions in superlattices and multilayers. Time dependent pattern formation in cases where misfit locations are pinned at the epitaxial interface.

434. THE ORGANIC CHEMISTRY OF CONDUCTING POLYMERS

L. M. Tolbert
Dept. of Chemistry
Phone: (404) 894-4002

$101,000 03-1

Synthesis of conducting polymers by forming charge carriers directly by deprotonation of the requisite carbon acids. The anions generated will be of two classes. The first class consists of discrete anions of known chain lengths whose magnetic and spectroscopic properties can be compared to those of the n-type soliton. The second class consists of anions embedded in an acetylene copolymer chain containing acidic methylene units. The transition to the conducting regime upon exhaustive deprotonation and polyene chain length extension will be determined. In related experiments, the role of radical anion disproportionation in formation of the carbanions will be investigated.

UNIVERSITY OF GEORGIA
Athens, GA 30602

435. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

W. M. Yen
Dept. of Physics & Astronomy
Phone: (404) 542-2485

$127,588 02-2

Comprehensive and detailed study of relaxation and energy transfer in and among optically excited states in disordered or amorphous systems and in certain ceramics. Application of new spectroscopic techniques to provide more fundamental understanding of prototypical transport processes, e.g. in rare earth-doped glasses or in mullites containing variable size crystallites. Advanced laser techniques, fluorescence line narrowing (FLN) and time-resolved FLN, measurement of coherent optical transients, photoacoustic and photocaloric methods, far infrared study using a free electron laser. Measurement and analysis of linewidths and lineshapes and of their temperature dependence, testing of models for the underlying mechanisms (e.g., ion-phonon interactions, two-level system model).

HARVARD UNIVERSITY
Cambridge, MA 02138

436. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

I. F. Silvera
Dept. of Physics
Phone: (617) 495-9075, 2872

$200,000 (10 months) 02-2

Investigation of the properties of quantum gases of spin-polarized atomic hydrogen and deuterium. Attempt to reach sufficient densities and low temperatures that these unusual gases will undergo Bose-Einstein condensation. Attempt to observe directly the surface atoms of spin-polarized hydrogen adsorbed on a helium film surface. Observe the onset of the expected superfluidity in the two-dimensional Bose-Einstein condensate.

HARVARD UNIVERSITY (continued)

437. SYNCHROTRON STUDIES OF X-RAY REFLECTIVITY FROM SURFACES

P. S. Pershan
Div. of Applied Science & Physics Department
Phone: (617) 495-3214

$162,500 (18 months) 03-3

Experimental study using glancing angle X-ray scattering to determine surface and near surface structure and density profiles. Pure liquid metals and alloys with melting temperatures no higher than lead (327C) will be examined in the initial phase. Ultra high vacuum equipment will be used to mantain clean surfaces. In addition, specular reflectivity of X-rays will be used to investigate the physical processes by which liquids deposit on solid surfaces.

UNIVERSITY OF HOUSTON
Houston, TX 77004

438. DIFFRACTION STUDIES OF THE STRUCTURE OF GLASSES AND LIQUIDS

S. Moss
Dept. of Physics
Phone: (713) 749-2840

$250,000 02-1

Development of a dedicated glass and liquid neutron diffractometer for use at the Intense Pulsed Neutron Source (IPNS) of Argonne National Laboratory with support and collaboration with Argonne. Design will optimize the need for required resolution and the ideal angular range appropriate to both high and low momentum transfer. High intensity, unique instrument. Usable wavelength range from 0.1 to 4 Angstroms with the solid methane moderator at 30 Kelvin temperature. Provide greater real space resolution. Structure and modeling of amorphous silicon, germanium, Si-Ge alloys with hydrogen. Tailoring of band gap state. Neutron studies of the glass transition. Structure of amorphous melanin, a biopolymer. Structure of SiO_2, SnO_2, and IrO_2.

IBM
Almaden Research Center
650 Harry Road
San Jose, CA 95120-6099

439. SEGMENTAL INTERPENETRATION AT POLYMER-POLYMER INTERFACES

Thomas P. Russell
Research Division
Phone: (408) 927-1080

$116,433 03-2

Study of segment density distributions at polymer-polymer interfaces using electron microscopic, small angle X-ray scattering, small angle neutron scattering and solid state polarization transfer NMR techniques. Investigate incompatible polystyrene-polymethylmethacrylate mixtures with corresponding copolymers that serve as compatibilizing agents. Combine results from the above four different techniques on identical speciments such that a detailed picture of segment density distribution of polymers and copolymers at the interface is determined. These polymer blends to be studied as a function of the molecular weight and composition.

INDIANA UNIVERSITY
Bloomington, IN 47402

440. HIGH-RESOLUTION ELECTRON ENERGY LOSS STUDIES OF SURFACE VIBRATIONS

L. L. Kesmodel
Dept. of Physics
Phone: (812) 335-0776

$ 98,000 02-2

Investigation of surface vibrational properties on metal and semiconductor surfaces with and without adsorbed overlayers. The experimental method employed is high-resolution electron energy loss spectroscopy (EELS) at an energy of 3-7 meV. Detailed surface phonon dispersion information to be obtained on copper, palladium, aluminum, and silicon with and without adsorbates such as hydrogen, oxygen, and sulfur. Results to be compared with realistic theoretical models of surface phonon dispersion and inelastic electron scattering in collaboration with theorists.

JOHNS HOPKINS UNIVERSITY
Baltimore, MD 21218

441. INVESTIGATION OF THE PROCESSES CONTROLLING THE FLAME GENERATION OF REFRACTORY MATERIALS

J. L. Katz
Dept. of Chemistry Engineering
Phone: (301) 338-8484

$83,844 01-3

Fundamental study of nucleation, growth and agglomeration of fine particles generated in flames. Correlation of gas phase species concentration with these processes and resultant particle sizes. Absorption and other spectroscopic methods utilized to follow gas phase species concentrations. Materials studied include silica, titania, alumina and germania.

KANSAS STATE UNIVERSITY
Manhattan, KS 66506

[redacted] MAGNETIC STUDIES OF IRON RARE-EARTH METALLOID ALLOYS

G. C. Hadjipanayis
Dept. of Physics
Phone: (913) 532-6786

$ 23,640 02-2

Investigation of the new iron rare-earth metalloid alloys with high potential for permanent magnetic applications including $Fe_{77}R_{15}M_8$ and $Fe_{82}R_{12}M_6$ where R is primarily a rare-earth and M is a metalloid such as B, C, and Si. Main emphasis on preparation techniques, correlation of magnetic properties of sputtered films with sputtering parameters, exploration of dependence of the magnetic properties on the electronic factors and atomic spacings in Fe-Nd-B alloys, and a detailed study of the relationship of microstructure, secondary phases and defects on the magnetization reversal and hysteresis. Work in collaboration with the University of Nebraska.

UNIVERSITY OF KENTUCKY
Lexington, KY 40506

443. MICROSCOPIC PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE INTERCALATION COMPOUNDS

P. C. Eklund
Dept. of Physics and Astronomy
Phone: (606) 257-6725

$ 27,000 02-2

Investigation of physical and chemical properties of well-staged graphite intercalation compounds (GIC). Sample synthesis via vapor phase and electrochemical intercalation, characterization (e.g., staging & in-plane order) using X-ray diffraction and Raman spectroscopy. Electronic transport and optical properties, lattice structural and dynamical properties of donor- and acceptor-type GIC's. Investigation of ion-assisted-deposition to be explored with significant new capital equipment purchased by the University of Kentucky.

444. STRUCTURE AND CATALYTIC ACTIVITY OF DISPERSED METAL PARTICLES AND METAL SURFACES

P. J. Reucroft
Dept. of Metallurgical Engineering and Material Science
Phone: (606) 257-8723
R. J. De Angelis
Dept. of Metallurgical Engineering and Material Science
Phone: (606) 257-3238

$105,300 (18 months) 03-3

Detailed structural and compositional characterization of metallic catalyst particles dispersed on porous oxide supports. Techniques such as analytical electron microscopy, X-ray diffraction, and energy dispersive and ion scattering spectroscopies will be used to examine the dispersed metal catalysts at various stages in their preparation to elucidate the role of strong and weak metal-support interactions on particle morphological development and particle thermal stability.

LEHIGH UNIVERSITY
Bethlehem, PA 18015

445. ANALYTICAL ELECTRON MICROSCOPY OF CATALYST PROMOTERS, POISONS, AND ACTIVE SPECIES

C. E. Lyman
Dept. of Metallurgy and Materials Engineering
Phone: (215) 758-4249

$ 79,981 01-1

Application of analytical, high resolution, controlled atmosphere, and high voltage electron microscopies to understand mechanisms of catalyst promotion and poisoning, and to locate particular species with respect to crystallographic site and surface topographic specifics in the support phase. Systems of interest include the Cu/ZnO and Cs/MoS_2 catalyst systems, Cs promoters, and Tl poisons. Near edge fine structure electron energy loss spectroscopy.

[illegible] ANALYTICAL ELECTRON MICROSCOPY STUDIES OF INTERFACES AND PHASE TRANSFORMATIONS IN ZIRCONIA CERAMIC SYSTEMS

M. R. Notis
Dept. of Metallurgy and Materials Science
Phone: (215) 758-4225
D. B. Williams
Dept. of Metallurgy and Materials Science
Phone: (215) 861-4220
C. E. Lyman
Dept. of Metallurgy and Materials Science
Phone: (215) 861-4249

$144,000 01-1

Structural studies of solid-state phase transformations and phase equilibria in binary and ternary ceramic systems which have potential for transformation toughening. Crystal structure and microchemistry determination by analytical electron microscopy (AEM), convergent beam electron diffraction (CBED), and high-resolution electron microscopy (HREM). Interphase interface structure and microchemistry in ZrO_2-$CaZrO_3$, ZrO_2-$SrZrO_3$, ZrO_2-NiO, ZrO_2-MgO, ZrO_2-Y_2O_3, and ZrO_2-mullite. AEM studies of stabilized cubic ZrO_2 systems to confirm existence of microdomains of ordered cations and anion vacancies. AEM, CBED, and HREM studies of phase transformations in $ZrO_2Y_2O_3$-TiO_2, and ZrO_2-MgO-TiO_2 systems.

LEHIGH UNIVERSITY (continued)

447. THE EFFECT OF POINT DEFECTS ON STRUCTURAL PHASE TRANSITIONS

J. Toulouse
Dept. of Physics
Phone: (215) 758-3960

$ 64,000 01-1

Study of the coupling of the Li defect to the B_{1g} soft phonon mode in MnF_2:Li and MgF_2:Li by Raman scattering and infrared absorption. Measurement of ultrasonic attenuation as a function of temperature from 4.2K so as to estimate the coupling of the Li defect relaxation to the B_{1g} soft phonon mode. Raman frequency shift, acoustic and dielectric measurements in $KMnF_3$:Li at temperatures spanning the cubic-tetragonal phase transition so as to identify the Li defect. Neutron scattering measurements in the constant Q-mode and as a function of temperature in Q range centered on the transition temperature with the triple axis spectrometer at the BNL-HFBR. Similar ultrasonic, Raman, and neutron scattering studies on $KTa(Nb,Sc)O_3$ and $PbZr(Sc,Mg)O_3$.

448. CORROSION FATIGUE OF IRON-CHROMIUM-NICKEL ALLOYS: FRACTURE MECHANICS AND CHEMISTRY

R. P. Wei
Dept. of Mechanical Engineering and Mechanics
Phone: (215) 758-3587

$165,000 01-2

Characterization and understanding of corrosion fatigue crack growth in austenitic stainless steels in aqueous environments. Influence of mechanical and chemical processes. Examination of microstructural influences. Growth of short cracks at low growth rates. Identify and quantify changes in crack-tip chemistry with changes in loading and environmental variables. Assess the role of crack closure in influencing the crack-tip environment and the effective crack driving force. Use of a 4-electrode in situ fracture technique.

[redacted]. [redacted]IN ORIENTED [redacted] BICRYSTALS CONTAINING BORON

Y-T. Chou
Dept. of Metallurgy and Materials Engineering
Phone: (215) 758-4235

$ 93,000 01-3

Measurement of grain boundary diffusion coefficients in B doped and undoped [001]/[100] tilt bicrystals of Ni_3Al. Preparation of such crystals.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, MA 02139

[redacted]

[redacted]alluffi
Dept. of Materials Science and Engineering
Phone: (617) 253-3349
P. D. Bristowe
Dept. of Materials Science and Engineering
Phone: (617) 253-3326

$468,273 01-1

A broad-based, fundamental investigation of the structure and properties of grain boundaries consisting essentially of combined computer simulation and experimental attacks on the problem of determining the atomic structure and corresponding properties of high-angle grain boundaries. Materials studied include Ag, Al, and Ge. Experimental techniques employed include X-ray diffraction, high-resolution and conventional electron microscopy and computer simulation.

451. BRITTLE-TO-DUCTILE TRANSITION IN CLEAVAGE FRACTURE

A. S. Argon
Dept. of Mechanical Engineering
Phone: (617) 253-2217

$126,433 01-2

Investigate the rate controlling processes that control the brittle-to-ductile transition in cleavage fracture, namely (a) the emission of dislocations from atomically sharp cracks, (b) the moving away from the crack tip of the emitted dislocations against strong lattice drag. Instrumented cleavage crack propagation experiments at several temperatures to determine the critical velocities below which the cracks become abruptly arrested in LiF, Fe-3%Si, W, MgO, Si, and Zn--all in either nearly perfect form, or containing some strongly misfitting solute that can be used to lock existing dislocations. Dislocation arrangements investigated by etching, X-ray topography, and TEM. Experimental velocity dependence of the brittle-to-ductile transition temperature compared with improved crack tip emission models. Quasi-static experiments to explore dislocation mobility away from the crack tip as a function of temperature and loading rates to determine the dependence of the T_{B-D} on loading rate. The experiments on Fe-3%Si and W with constant stress intensity geometry compared with models of time dependent crack-tip shielding governed by dislocation mobility.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

452. [redacted]

Y-M. Chiang
Dept. of Materials Science and Engineering
Phone: (617) 253-6471

$115,400 01-2

Investigation grain boundary nonstoichiometry and its relation to grain boundary mobility and grain boundary effects on electrical conductivity. Systems to be examined are lead-zirconium-titanate, lead-lanthanum-zirconium-titanate, the superconducting cuprates, stronitium and barium titantates. DC conductivity and AC frequency-dependent complex impedance measurements will monitor electrical behavior which will be correlated with the stoichiometry and composition of grain boundaries as determined by STEM, light-element microanalysis and Auger spectroscopy.

453. SUPERCONDUCTIVITY AND MAGNETISM IN RAPIDLY SOLIDIFIED PEROVSKITES

G. Kalonji
Dept. of Materials Science and Engineering
Phone: (617) 253-6863
R. O'Handley
Dept. of Materials Science and Engineering
Phone: (617) 253-6913

$175,000 01-3

Investigation of magnetic and superconducting behavior in series $GdBa_2(Cu_{1-x}Fe_x)O_7$ and $La_{2-y}Sr_y(Cu_{1-x}Fe_x)O_4$ from strongly magnetic limit to strongly superconducting limit. Magnetic susceptibility and Mossbauer measurements used to determine spin states and valences. New magnetic and superconducting phases fabricated by conventional and rapid solidification processing techniques.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

454. STRUCTURAL DISORDER AND TRANSPORT IN TERNARY OXIDES WITH PYROCHLORE STRUCTURE

H. L. Tuller
Dept. of Materials Science and Engineering
Phone: (617) 253-6890

$110,000 01-3

Relationship of electrical and optical properties to the defect structure in ternary compounds with a pyrochlore structure. Characterization of AC complex impedance of rare earth titanate and zirconate pyrochlores under conditions of controlled composition, temperature, and chemical environment. Optical absorption and emission measurements to monitor the degree of disorder. Preparation of single and polycrystalline samples of known cation-anion ratio by pyrolysis of metal-citrate complex precursors. Complementary sample characterization by thermogravimetric analysis, X-ray diffraction, and Raman spectroscopy. Specific pyrochlores to be investigated are $Gd_2Zr_2O_7$ and solid solutions in the $Gd_2Zr_2O_7$-$Dy_2Zr_2O_7$ and $Gd_2Zr_2O_7$-$Gd_2Ti_2O_7$ systems.

[redacted] MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS

G. J. Yurek
Dept. of Materials Science and Engineering
Phone: (617) 253-3239

$210,000 01-3

Investigation of the mechanisms of oxidation and oxidation/sulfidation of metals and alloys at elevated temperatures. Emphasis on the formation of protective refractory oxide scales such as Cr_2O_3, Al_2O_3 and/or SiO_2 and on factors controlling scale degradation in gas mixtures having high rations of sulfur to oxygen activity. In addition, influences of very fine-grained microstructures of the substrate (via rapid solidification processing) on oxide formation (and subsequent breakdown) and the effects on oxidation resistance associated with foreign ions at oxides scale grain boundaries will be examined.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

456. IRRADIATION DAMAGE MICROSTRUCTURES IN NUCLEAR CERAMICS WITH APPLICATION IN FUSION ENERGY TECHNOLOGY AND NUCLEAR WASTE DISPOSAL

L. W. Hobbs
Dept. of Materials Science and Engineering
Phone: (617) 253-6835

$118,460 01-4

Fundamental research to characterize the irradiation stability and radiation damage regarding microstructures of crystalline ceramic solids with application to nuclear energy production and disposal of high-level nuclear waste.

The principal experimental mode of investigation is transmission electron microscopy. Specific emphasis will be on (1) radiolysis and Frenkel pair stabilization in BeO, (2) perovskite metamictization by ion implantation, (3) nanostructure of pyrochlore-phase ceramics, and (4) computer simulation of network silicates.

[redacted]. IDENTIFICATION OF NITRIDING MECHANISMS IN HIGH PURITY REACTION BONDED SILICON NITRIDE

J. S. Haggerty
Dept. of Materials Sciences and Engineering
Phone: (617) 253-2129

$121,622 01-5

Nitriding studies on silicon powders and single crystals to identify the rate controlling mechanisms and examination of samples along the reaction path to elucidate the relationships between reaction kinetics and microstructural features. In-house preparation and characterization of laser synthesized silicon powder for reaction bonded silicon nitride (RBSN) experiments. Investigation of nitriding process will determine effect of solvent exposure, partial densification, variations in gas composition, temperature gradients, particle size, particle distribution, and temperature cycles. Experimental data to elucidate silicon nitride layer formation, heterogeneous reaction rate dependence on particle coarsening, vapor phase species, and gaseous diffusion through pore structure of solid.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

458. THE MATHEMATICAL MODELLING OF ARC WELDING OPERATIONS

J. Szekely
Department of Materials Science and Engineering
Phone: (617) 253-3236
$106,236 01-5

This project carries out mathematical modelling with the main focus on: study of spot welding, use of three-dimensional models to study continuous welding, assessment of the effect of the thermal history of the system on the microstructure of the welds produced and initiate an assessment of weldpool free surface deformation and surface waves, and their effect on weld quality. The modelling efforts interact with an experimental program at Oak Ridge National Laboratory.

459. SUBMICRON LAYERS OF Nb-Al

S. Foner
Francis Bitter National Magnet Laboratory
Phone: (617) 253-5572
$130,460 02-2

Basic studies of thin layers of superconducting materials to understand the limits on critical transition temperature, critical current and upper critical field. Determine optimum layer thickness for complete conversion to A15 structure. Examine possible elemental additions to improve the transition temperature and assist in approaching stoichiometry. Microcomposite ultrathin film multilayers for increased mechanical strength.

460. IMPROVEMENT IN HIGH MAGNETIC FIELD BEHAVIOR OF VANADIUM-GALLIUM SUPERCONDUCTORS BY ENHANCEMENT OF SPIN-ORBIT SCATTERING

R. H. Meservey
Francis Bitter National Magnet Laboratory
Phone: (617) 253-5578
P. M. Tedrow
Francis Bitter National Magnet Laboratory
Phone: (617) 253-0281
$ 25,000 02-2

Development of a tunneling technique to measure density of states in V_3Ga. Determination of spin-orbit scattering in this material. Understand the relation between spin-orbit scattering and critical magnetic field in this superconductor. Spin-polarized tunneling.

MIAMI UNIVERSITY
Oxford, OH 45056

461. INVESTIGATION OF MAGNETIC ANISOTROPY AND SPIN WAVE MODES IN TRANSITION METAL MULTILAYERS

M. J. Pechan
Dept. of Physics
Phone: (513) 529-4518

$ 38,000 02-2

Investigation of magnetic multilayers (Ni/Mo and Ni/V) using ferromagnetic resonance. Measurements of the frequency dependence of the anisotropy and spectral lineshapes. Collaborators are fabricating and structurally characterizing the multilayer samples for study.

MICHIGAN STATE UNIVERSITY
East Lansing, MI 48824

462. SOFTENING MECHANISMS AND MICROSTRUCTURAL INSTABILITIES DURING HIGH TEMPERATURE LOW CYCLE FATIGUE OF NI, NI_3AL AND THEIR METAL MATRIX COMPOSITES

G. Gottstein
Dept. of Metallurgy, Mechanics, and Materials Science
Phone: (517) 353-9767

$ 94,918 01-2

Investigation into the mechanisms that govern the microstructural development during high-temperature low-cycle fatigue of Ni, Ni_3Al and their metal matrix composites with particular emphasis on grain boundary motion and realignment, dynamic recrystallization and grain growth. Analysis of dislocation structures, sub-boundary misorientation and internal stresses at sub-boundaries and at heterogeneous interfaces. Development and control of dynamically recrystallized structures, grain size and texture. Effect of boron. Characterization techniques include mechanical testing, TEM, STEM, X-ray pole figure measurements, X-ray micro-Laue diffraction and Auger spectroscopy.

MICHIGAN TECHNOLOGICAL UNIVERSITY
Houghton, MI 49931

[redacted]. EFFECTS OF GRADIENTS ON [redacted] STABILITY

S. Hackney
Dept. of Metallurgical Engineering
Phone: (906) 487-2170

$124,414 01-1

Study of diffusion-induced grain boundary migration from a microscopic point of view. Time and concentration dependence of the initiation of migration. Grain boundary morphology studies by in-situ hot stage electron microscopy. Effects of diffusion-induced grain boundary migration on the morphological development of second phase precipitates. Thermotransport-induced grain boundary migration. Effects of elastic strain gradient on interface migration.

464. STRESS CORROSION CRACKING AND METAL INDUCED EMBRITTLEMENT

L. A. Heldt
Dept. of Metallurgical Engineering
Phone: (906) 487-2630

$ 99,000 01-2

Parallel studies of stress corrosion cracking (SCC) and metal induced embrittlement (MIE), with emphasis on the kinetics of the cracking process and the nature of the chemical interactions causing embrittlement. Experimental tasks include (1) surface chemical analysis near the tips of SCC and MIE cracks, (2) simulation of the solution chemistry within SCC cracks, (3) measurement of crack propagation velocities as influenced by the chemical/electrochemical environment, stress intensity, and temperature, and (4) detailed microscopic studies of resultant fracture surfaces.

MICHIGAN TECHNOLOGICAL UNIVERSITY (continued)

465. THEORY OF DEFECTS IN NON-METALLIC SOLIDS

A. B. Kunz
Dept. of Physics
Phone: (906) 487-2277
D. R. Beck
Dept. of Physics
Phone: (906) 487-2019

$ 96,040 02-3

Calculations for impurities in oxides and other ceramic or ionic solids to support studies of effects of point defects on mechanical properties and electronic structure. Fully self-consistent correlated electronic structure computation for a central cluster containing the impurity combined with shell-model calculation of host polarization and distortion. Absolute energies of the impurity ions for each of their pertinent charge states in a given host are calculated, and the electronic structure and lattice ion relaxations are determined self-consistently to obtain interatomic interactions adequate for a broad range of applications (mechanical properties as well as electronic structure). Emphasis on quantum mechanical treatment of cases in which conventional empirical methods are inadequate. Various defect and impurity centers, mainly in oxides, including transition metal ions, anion defects, such as H, F, and C will be the subject of specific calculations.

UNIVERSITY OF MICHIGAN
Ann Arbor, MI 48109

466. MICROMECHANICAL AND MICROSTRUCTURAL STUDIES OF CERAMIC SUPERPLASTICITY

I-W. Chen
Dept. of Materials Science and Engineering
Phone: (313) 763-6661

$110,000 01-2

Pressure-aided superplasticity in single and poly-phase ceramics. Experiments with dense isostructural ceramics (ZrO_2-CeO_2, CaF_2-SrF_2, $BaTiO_3$, and $BaTiO_3$-TiO_2) employed (1) to define constitutive relations under stress, (2) to determine pressure effects on ductility and (3) to monitor concurrent deformation-induced and deformation-enhanced microstructural and microchemical evolutions that impact the micromechanics of ceramic superplasticity. Testing modes include tension-compression, tension-torsion and pressure-assisted tension-compression. Grain growth, cavitation, phase and compositional segregation will be constantly examined.

UNIVERSITY OF MICHIGAN (continued)

467. THE ROLE OF [redacted] CHARACTER IN THE ENVIRONMENTALLY-ASSISTED INTERGRANULAR CRACKING MECHANISM OF NICKEL-BASED ALLOYS

G. S. Was
Dept. of Nuclear Engineering
Phone: (313) 763-4675

$157,622 01-2

The objective of this program is to determine the role of grain boundary character in the mechanism of environmentally-assisted intergranular cracking in nickel-base alloys. The effects of boundary misorientation; inclination; precipitate density distribution; precipitate composition, structure and coherency; and major and minor element content will be studied. Research tasks include chemical and structural characterization of the grain boundary, atomistic modeling of grain boundary processes, and stress corrosion cracking and hydrogen embrittlement testing and comparison with model results. Experiments on both laboratory and commercial heats of Ni-Cr-Fe alloys. The ultimate goal is to control grain boundary structure to resist intergranular cracking.

468. THE STRUCTURAL BASIS FOR FATIGUE INITIATION IN GLASSY POLYMERS

A. F. Yee
Dept. of Materials Science and Engineering
Phone: (313) 764-4312

$116,143 01-2

Fatigue initiation in glassy polymers, including structural changes which precede the initiation of visible cracks and crazes. Relationship between low amplitude cyclic stresses and polymer aging. Applications of small angle X-ray scattering (SAXS) and position annihilation techniques (PAT) to the characterization of the temporal evolution of structural change. Relaxation behavior to be used to predict craze initiation.

UNIVERSITY OF MICHIGAN (continued)

[redacted] INVESTIGATIONS ON THE MBE GROWTH AND PROPERTIES OF AlGaInAs/InP AND InGaAs-InAlAs SUPERLATTICES

P. K. Bhattacharya
Dept. of Electrical Engineering and Computer Science
Phone: (313) 763-6678
R. Gibala
Dept. of Materials Science and Engineering
Phone: (313) 763-4970

$135,055 01-3

Molecular beam epitaxial growth and in situ RHEED studies of single layers, heterostructures, and superlattices of In containing ternary and quaternary compounds and superlattices lattice matched to InP. Investigation of the role of growth conditions (substrate temperature, arsenic specie, fluxes) on the surface kinetics operative for 2-dimensional layer-by-layer growth. Computer simulations based upon Monte Carlo methods. Structural characterization of crystals and interfaces by TEM, CBED, HVEM, XRD, and etching. Optical and impurity characterization by high-resolution Raman, photoluminescence, high magnetic field FTIR spectroscopies. Electrically active defect characterization by DLTS.

[redacted] A STATISTICAL MECHANICS STUDY OF SOLID-SOLID [redacted]

D. J. Srolovitz
Dept. of Materials Science and Engineering
Phone: (313) 936-1740

$200,000 01-3

Theoretical methods and computer simulations to investigate the structure and thermodynamic properties of grain boundaries and other interfaces in pure metals, alloys (solid solution and ordered), and two-phase systems. Applications of a statistical mechanical density-functional theory and Monte Carlo calculations in the grand canonical ensemble.

UNIVERSITY OF MICHIGAN (continued)

471. THEORY OF NON-EQUILIBRIUM GROWTH

L. M. Sander
Dept. of Physics
Phone: (313) 764-4471
R. Savit
Dept. of Physics
Phone: (313) 764-3426

$194,050 02-3

Theoretical proposal at the forefront of a recent approach to understanding the relationships between growth mechanisms, structure, and properties of nonequilibrium systems, such as smoke, colloids, deposition of vapors and electrolytes which have been shown to give rise to scale invariant fractal-like structures. Objects of this type have a morphology which lies between conventionally studied crystalline geometry (with a very high degree of regular symmetry) and the amorphous state (with no special symmetry). The unique properties of this kind of matter can be traced to the fact that it posses an invariance property not shared by either crystalline or amorphous matter; that of non-trivial scale-invariance. That is, the systems "look" the same on all length scales and scale with a generally non-integer dimension. The behavior of various kinds of random walks on these fractal clusters as well as the behavior of equilibrium statistical spin systems defined on the clusters will be of interest for helping scientists understand the dynamics of such random scale-invariant objects. The principal investigators expect to rely heavily on both analytical techniques and numerical simulations in this work.

UNIVERSITY OF MINNESOTA
Minneapolis, MN 55455

472. MICROMECHANICS OF BRITTLE FRACTURE: ACOUSTIC EMISSION AND ELECTRON CHANNELING ANALYSES

W. W. Gerberich
Dept. of Chemical Engineering and Materials Science
Phone: (612) 625-8548

$ 91,224 01-2

Research to address (1) crack dynamics and inherent plasticity effects, (2) ligament contributions to fracture resistance and (3) micromechanics of final instability. Polycrystalline and single crystal materials investigated as a function of temperature, grain size and material thickness. Materials: high-strength, low-alloy (HSLA) steel, Fe-3wt%Si and zinc single crystals. Techniques include detailed fractography, acoustic emission, selected area channeling pattern (SACP) evaluation, cleavage modeling, TEM, impact and mechanical studies.

UNIVERSITY OF MINNESOTA (continued)

473. A STUDY OF SCALE CRACKING AND ITS EFFECTS ON OXIDATION AND HOT CORROSION OF METALS AND ALLOYS

D. A. Shores
Dept. of Chemical Engineering and Materials Science
Phone: (612) 625-0014

$200,000 01-3

Study and elucidation of the mechanisms of oxidation and hot corrosion of selected metals and alloys through an interdisciplinary team approach in which the phenomena of growth stresses, thermal stresses and scale cracking are examined. Theoretical modeling of isothermal, athermal, and time-dependent growth stresses. In situ experimental measurement of scale stresses and experimental determination of the occurrence of scale cracking under various corrosive conditions. Scale cracking related to measured and calculated stresses. Experimental techniques include X-ray diffraction, acoustic emission, thermogravimetric analysis, cyclic voltammetry, chronopotentiometry, and optical/electron microscopy.

474. MODELING AND EXPERIMENTAL STUDIES OF OXIDE COVERED METAL SURFACES TIO_2 ON TI: A MODEL SYSTEM

W. H. Smyrl
Dept. of Chemical Engineering and Materials Science
Phone: (612) 625-0717

$372,425 01-3

Studies intended to characterize the ordered growth of oxide on titanium. Influence of growth conditions on the structure and texture of oxide films. Reflection, transmission, and scanning electron microscopy will be used. Local electronic properties of oxide films investigated by photoelectrochemical microscopy. Calculation of the electronic structure of various defects in thin films of titanium oxide. Vibrational Raman spectroscopy used as a diagnostic probe of the growth and structure of titanium oxide thin films. Determination of the concentration and identity of structural defects in the oxide lattice. X-ray scattering and X-ray absorption spectroscopy made in situ under potential control. EXAFS used to determine geometric structure and XANES used to obtain information on chemical environment. X-ray scattering used to examine long-range order and structure of passive films.

UNIVERSITY OF MINNESOTA (continued)

475. VERY LOW TEMPERATURE STUDIES OF HYPERFINE EFFECTS IN METALS

W. Weyhmann
School of Physics and Astronomy
Phone: (612) 373-5481

$ 78,000 02-2

Hyperfine enhanced nuclear magnetism of rare earth alloys. Temperatures less than 1 milliKelvin. Properties measurements: heat capacity, magnetization, electrical resistance, frequency dependent complex susceptibility, and magnetostriction. Materials of praseodymium-copper and praseodymium-nickel ($PrCu_6$, $PrNi_5$) in single crystal form and in diluted compounds. Dilute local moments; nuclear orientation measured on very dilute magnetic ion systems. Itinerant ferromagnetism.

UNIVERSITY OF MISSOURI/COLUMBIA
Columbia, MO 65211

476. INTRINSIC AND EXTRINSIC ENERGY STATES OF SEMICONDUCTORS AND HETEROSTRUCTURES USING NOVEL TECHNIQUES

H. R. Chandrasekhar
Dept. of Physics and Astronomy
Phone: (314) 882-6086

$ 25,334 (20 months) 02-2

Modulated reflectance and photoemission spectroscopy of GaAs-$Al_xGa_{1-x}As$ semiconductor material. Donor and acceptor impurity states will be studied. Semiconducting superlattices with quantized energy levels due to hole or electron confinement in potential wells determined. Photoluminescence, photoreflectance and Raman scattering techniques coupled with diamond anvil cell high pressure techniques.

UNIVERSITY OF MISSOURI (continued)

477. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION

W. B. Yelon
Dept. of Physics
Phone: (314) 882-5236

$ 75,492 02-2

Development of new Mossbauer techniques with a microfoil electron detector, LiF monochromator, and high intensity sources. Accurate measurement of the Mossbauer isomer for the 46.5 keV transition in ^{183}W. Test of time reversal invariance in gamma emission accompanying nuclear decay to an order of magnitude greater accuracy than previously attained. Resonance scattering from TaS_2-1T that permits study of the charge density wave phenomena in this material. Thermal diffuse scattering and Debye-Waller factor scattering between temperatures of 77 and 295 Kelvin (room temperature). Attempted measurement of inelastic scattering, resulting from one phonon processes near the edge of the Brillouin zone.

UNIVERSITY OF MISSOURI/KANSAS CITY
1110 E. 48th Street
Kansas City, MO 64110

478. THEORETICAL STUDIES ON THE ELECTRONIC STRUCTURE AND PROPERTIES OF COMPLEX CERAMIC CRYSTALS AND GLASSES

W-Y. Ching
Dept. of Physics
Phone: (816) 276-2503

$121,356 01-1

Total energy electronic structure calculations on crystalline and vitreous ceramics. Studies of superconducting oxides, mixed-layer perovskites, ZrO_2, α-quartz, β-Si_3N_4, α-Al_2O_3, α-Si_3N_4, various spinel-structured oxides, metallic and insulating glasses using a first-principles LCAO method. A sequential approach (1) performs accurate full-potential, self-consistent calculations of electronic structure and total energy of crystalline ceramics, (2) uses the direct-space orthogonal LCAO approach for spinels, (3) extracts interatomic potentials from key crystal calculations for phase stability and other thermodynamic property predictions.

UNIVERSITY OF MISSOURI/ROLLA
Rolla, MO 65401

479. CHARACTERIZATION OF ELECTRICALLY CONDUCTING OXIDES

H. U. Anderson
Dept. of Ceramic Engineering
Phone: (314) 341-4886

$145,000 01-3

Interrelationships between electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n- and p-type binary and ternary transition metal oxide, and superconducting layered perovskites. Focus on the influence of electric fields and oxygen activity gradients on oxide-electrode stability, oxygen transport through oxides, and dopant energy levels in oxides. Experimental techniques include thermogravimetric characterization, optical microscopy, X-ray and neutron diffraction, TEM, electrical conductivity, Seebeck coefficient studies, thermally and optical stimulated current spectroscopy and deep level transient spectroscopy.

MONTANA STATE UNIVERSITY
Bozeman, MT 59717

480. STUDIES OF PIEZOELECTRIC POLYMERS

V. H. Schmidt
Dept. of Physics
Phone: (406) 994-6173

$ 45,964 03-2

Study of chain conformation, rotations, and other motions in the piezoelectric polymers polyvinylidene fluoride and its copolymer with trifluoroethylene by NMR and optical techniques. Pressure and temperature dependence on the nonferroelectric to ferroelectric phase transitions. NMR of deutreated samples and optical studies involving birefringence, small angle light scattering, and Brillouin scattering to measure degree of chain alignment and sound velocity and attenuation as affected by polymer processing and by temperature and pressure induced phase transitions.

UNIVERSITY OF NEBRASKA
Lincoln, NE 68588-0111

[redacted] FUNDAMENTAL MAGNETIC STUDIES OF IRON-RARE-EARTH-METALLOID ALLOYS

D. J. Sellmyer
Dept. of Physics
Phone: (402) 472-2407

$ 56,849 02-2

Investigation of the new iron-rare-earth-metalloid alloys with high potential for permanent magnetic applications including $Fe_{77}R_{15}M_8$ and $Fe_{82}R_{12}M_6$ where R is primarily a rare-earth and M is a metalloid such as B, C, and Si. Main emphasis on preparation techniques, correlation of magnetic properties of sputtered films with sputtering parameters, exploration of dependence of the magnetic properties on the electronic factors and atomic spacings in Fe-Nd-B alloys, and a detailed study of the relationship of microstructure, secondary phases and defects on the magnetization reversal and hysteresis. Work in collaboration with Kansas State University.

UNIVERSITY OF NEVADA
Reno, NV 89557

482. ENERGY TRANSFER BY TRIPLET EXCITON MIGRATION IN POLYMERIC SYSTEMS

R. D. Burkhart
Dept. of Chemistry
Phone: (702) 784-4133

$100,000 03-1

Studies of triplet-triplet annihilation and rate of triplet exciton diffusion in polymers. Direct excitation of ground state polymer chromophores to lowest triplet state through dye laser pumping. Investigation of the rate of triplet exciton migration in polymers having pendant groups which are sterically crowded and non-planar to assess the extent to which structural modifications can influence rates of exciton migration.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 97131

483. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE COMPLEX Nb-Ta-Ti OXIDES, PHOSPHATES, AND SILICATES

R. C. Ewing
Dept. of Geology
Phone: (505) 277-4163

$105,300 01-1

Investigation of metamict mineral/ion implanted ceramics concerning (1) periodic aperiodic reaction paths, (2) retained structures in fully damaged materials and (3) recrystallization products accompanying the annealing process. Techniques include X-ray diffraction, high resolution transmission electron microscopy (HRTEM) and extended X-ray absorption fine structure spectroscopy (EXAFS) and near-edge spectroscopy (XANES). Ta-rich pyrochlores, ABO_4 structured materials zircon ($ZrSiO_4$), thorite ($ThSiO_4$) and its polymorph huttonite, monazite ($CePO_4$) and fergusonite ($YNbO_4$) plus titanite ($CaTiOSiO_4$) are to be examined in their natural and synthesized states.

484. ADSORPTION STUDIES AT A SOLID-LIQUID INTERFACE

J. A. Panitz
Dept. of Physics
Phone: (505) 277-0607

$209,993 01-1

Adsorption phenomena at a solid-liquid interface. Monolayer films and multilayer structures formed on metal and semiconductor surfaces by Langmuir-Blodgett and simple diffusive adsorption from aqueous solution. Surface morphology, adsorbate conformation, and chemical analysis of interface mapped in high vacuum on a subnanometer scale using a new instrument that combines high-resolution transmission electron microscopy with imaging atom-probe mass spectroscopy. Vitreous ice, formed from the native environment, used to cryoprotect the interface, allowing the embedded interface and the species adsorbed on its surface to be transferred into high vacuum for analysis without modification or damage.

UNIVERSITY OF NEW MEXICO (continued)

485. ICOSAHEDRAL BORON-RICH SOLIDS AS VERY-HIGH TEMPERATURE THERMOELECTRICS AND SEMICONDUCTORS

C. L. Beckel
Dept. of Physics
Phone: (505) 277-2449
V. M. Kenkre
Dept. of Physics
Phone: (505) 277-2616
D. Emin
Dept. of Physics
Phone: (505) 277-8602

$176,000 (24 months) 02-3

Theoretical studies of boron-rich solids with structures typically consisting of boron icosahedra strongly linked by two or three atom chains, and stable to very high temperatures. Examples: pure and doped $B_{12}C_2$, $B_{12}P_2$, $B_{12}As_2$, and other compositions such as B_4C. Focus on test of theoretical models through prediction of electronic, vibrational, heat transfer and optical properties. Theoretical studies directed toward understanding and controlling these properties at a microscopic level. Polaron theory, cluster-based electronic calculation, classical force field calculations, transport of electronic and vibrational excitation by diffusion of extended excitations and/or by hopping of localized excitations. Soluble models of primary physical mechanisms. Quantitative theoretical descriptions, but generally not ab initio computation (due to complexity of the systems), with self-consistency both in electronic structure and of equilibrium geometry. Significant technological as well as scientific interest, primarily in potential use of borides in very-high temperature semiconductor and/or thermoelectric applications. Theoretical effort strongly interactive with a major experimental program involving SNL/A, JPL, and UNM.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE
New York, NY 10031

486. INVESTIGATIONS OF SURFACE COATINGS BASED ON SILICON AND NITROGEN: FROM AMORPHOUS Si TO SILICON NITRIDE

F. W. Smith
Dept. of Physics
Phone: (212) 690-6963

$112,865 01-3

Preparation of thin-film surface coatings by glow discharge of disordered alloys of silicon, nitrogen and hydrogen (α-Si_xN_{1-x}:H). Characterization using Auger depth profiling, measurements of density and optical constants (n, k, ϵ_1, and ϵ_2), IR spectroscopy and core-level spectroscopy. Valence band spectra and binding energy determinations using synchrotron radiation at the BNL NSLS.

487. DYNAMICS AND PATTERN SELECTION AT THE CRYSTAL-MELT INTERFACE

H. Z. Cummins
Dept. of Physics
Phone: (212) 690-6921

$120,000 02-2

Dynamics at the crystal-melt interface, especially the unexpected critical growth velocity for light scattering at the interface. Instabilities at the interface using videomicroscopy and image processing. Oscillations near the dendrite tip associated with the launching of side branches. Further development of the light scattering techniques to provide increased resolution and more accurate comparison with theory.

488. MAGNETIC PROPERTIES OF DOPED SEMICONDUCTORS

M. Sarachik
Dept. of Physics
Phone: (212) 690-6921

$110,000 02-2

A precise systematic study of the magnetic properties of homogeneous, well-characterized samples of heavily doped semiconductors as a function of impurity concentration across the metal-nonmetal transition. Faraday balance measurements as a function of temperature (from 1.25 K to 300 K) and of magnetic field (to 50 kG) to separate various contributions to the total susceptibility. The measurements will be extended to 50 mK and 190 kG at the National Magnet Laboratory. The role percolation has in the transition will be determined.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

489. TRANSPORT IN SMALL AND/OR RANDOM SYSTEMS

M. Lax
Dept. of Physics
Phone: (212) 690-6864, (201) 582-6527

$111,538 02-3

Theoretical research on transport and optical properties of semiconductor heterojunctions. Use of both numerical and analytical techniques, including some exact solutions of models. Monte-Carlo analysis of transport of phonons in GaAs films at sufficiently low temperatures that the film thickness is just several mean free paths. Electron-phonon interactions in a single quantum well. Electrons (or holes) in inversion layers or MOS structures. Noise in heterostructures and semiconductor lasers in the limit of small size.

CITY UNIVERSITY OF NEW YORK/QUEENS COLLEGE
Flushing, NY 11367

490. DIRECT SYNTHESIS AND OPTIMIZATION OF Fe-BASED, RARE-EARTH, TRANSITION METAL PERMANENT MAGNET SYSTEMS

F. J. Cadieu
Dept. of Physics
Phone: (718) 520-5000

$184,488 01-1

Prepare and characterize polycomponent metal films of $Nd_2Fe_{14}B$, and related $R_2Fe_{14}B$ systems, $(Sm + Ti)Fe_5$, $Sm(Ti,Fe)_2$, and $Sm_2(Co,Fe,Zr)_{17}$ under a variety of conditions by RF sputtering. Films made with and without a composition gradient along the length of the substrates. Selectively thermalized sputtering employed to yield highly textured and metastable structures to aid in the direct growth of crystallographically orientated samples. X-ray diffraction, X-ray fluorescence analysis and electron microprobe analysis will be employed to determine crystal structure and composition variations. High field magnetization and electron energy loss spectroscopy measurements on films with varying crystallographic texturing; selected magneto-optical measurements will be carried out.

STATE UNIVERSITY OF NEW YORK/BUFFALO
BUFFALO, NY 14214

491. CONSTRUCTION AND OPERATION OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

P. Coppens
Dept. of Chemistry
Phone: (518) 831-3911

$425,453 02-2

Construction and operation of the SUNY beam line at the National Synchrotron Light Source at Brookhaven National Laboratory. Relocated to X3, to provide X-ray optics and experimental stations: tunable monochromator, double focusing mirror, 6-circle diffractometer for crystallography, diffraction, spectroscopy, and reflectivity studies; additional Kratky collimator and two linear position-sensitive detectors for small and wide angle scattering; tunable monochromator for spectroscopy, standing waves, and reflectivity studies; additional ultra-high vacuum with conventional Low Energy Electron Diffraction (LEED) and Auger diagnostics for surface diffraction and surface standing wave studies. Participants from many State Universities of New York, Alfred University, Roswell Park Memorial Institutions, the University of New Orleans, and Allied Corporation. Research interests include, structure of materials, electronic structure of materials, surface physics, compositional analysis, and time-dependent biological phenomena.

STATE UNIVERSITY OF NEW YORK/STONY BROOK
Stony Brook, NY 11794

[redacted] [redacted] PROPERTIES AND CRYSTAL-GROWTH MECHANISMS

J. Q. Broughton
Dept. of Materials Science and Engineering
Phone: (516) 516-6754

$ 76,975 01-1

Use of computer simulation methods to examine synergistic effects of roughening and surface melting in crystal-vapor systems; mechanism of impurity incorporation in rapidly growing crystals; anisotropy of growth velocity with different crystal faces in crystal-melt systems; incidence of melt regions forming in grain boundaries at high temperatures; rough-smooth transitions observed in MBE grown crystal-vapor systems; influence of directional bonding (e.g., in network formers like Si) on interface width, growth velocity, impurity trapping, and roughening temperature.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

[redacted]. RESEARCH CONSORTIUM FOR X-RAY TOPOGRAPHY ON LINE X-19 AT NSLS

M. Dudley
Dept. of Materials Science and Engineering
Phone: (516) 689-8503

$ 89,711 (5 months) 01-1

Implementation of facilities and research for the Synchrotron Topography Project beamline X-19C at the National Synchrotron Light Source at Brookhaven National Laboratory under the auspices of a National Consortium headed by the SUNY Stony Brook group. The consortium is working on a wide range of problems where the special properties of synchrotron radiation are particularly suited, including: studies of the factors controlling elastic-plastic crack propagation, real-time slip initiation observations, quality assessment of crystal growth, mechanical integrity of thin film-substrate interfaces, thermal decomposition mechanisms for inorganic single crystals, in situ measurements of the film stresses accompanying film deposition for refractory metal silicides on silicon, detailed studies of the interaction of acoustic waves with microstructural constituents, morphology of pressure quenched CdS and X-ray topography and microradiography aimed at understanding high temperature deformation mechanisms of steels.

494. RADIATION EMBRITTLEMENT IN BCC METALS

S. Michael Ohr
Dept. of Materials Science and Engineering
Phone: (516) 632-8485

$116,950 01-4

Study the mechanism of radiation embrittlement in bcc metals by closely examining the relationship between the nature, the density, and the size distribution of defect clusters introduced by neutron irradiation and the mode of plastic deformation and fracture. Polycrystalline samples of molybdenum and niobium with controlled amounts of impurities, particularly carbon, irradiated at the LTNIF at temperatures between 4 and 500 K. The nature and size distribution of defect clusters determined as a function of neutron fluence, irradiation temperature, and impurity content by cold-transferring samples and performing TEM. Tensile samples irradiated simultaneously with the TEM samples. The extent of radiation hardening determined from the increase in yield stress. The sensitivity to radiation embrittlement measured in terms of the reduction in area and the strain to fracture. Neutron-irradiated samples deformed in an electron microscope to observe directly the motion of dislocations and the formation of dislocation channels as a function of neutron irradiation temperatures. In situ TEM fracture experiment to observe directly the difference in the way the defect clusters interact with cracks and the presence, or absence, of crack tip deformation during tensile deformation.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

495. ATOMIC AND ELECTRONIC STRUCTURE OF SURFACES AND CHEMISORBED LAYERS

F. P. Jona
Dept. of Materials Science and Engineering
Phone: (516) 246-7649, 6759

$146,195 02-2

Chemisorbed metal adsorbates on metal surfaces. Investigate structure with low energy electron diffraction (LEED). Determine electron band structure, including valence band shifts with layer thickness, with ultraviolet photoemission spectroscopy (UPS) on the U-7 beam line at the National Synchrotron Light Source at the Brookhaven National Laboratory. Alloy formation in gold-on-copper and palladium-on-copper. Surface reactivity in the gold-on-platinum and platinum-on-gold systems. Understand the process of alloy formation and chemisorption from correlation of the atomic and electronic structures.

496. X-RAY STUDIES OF STRAIN, INTERFACE AND IMPURITY IN SEMICONDUCTORS

Y. H. Kao
Dept. of Physics
Phone: (516) 632-8132

$ 95,000 02-2

X-ray techniques are employed to pursue a systematic study of short-range-order structure in semiconductors, including strained-layer superlattices, interface in heterojunctions, and ion-implanted impurities. Experimental methods are based on extended X-ray absorption fine structure (EXAFS), fluorescence-yield measurement of atomic profile (FLYMAP), and reflectivity measurements making use of synchrotron radiation at NSLS and CHESS.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

497. KINETICS OF PHASE SEPARATION IN POLYMER SOLUTIONS AND BLENDS

B. Chu
Dept. of Chemistry
Phone: (516) 246-7792

$ 95,000 03-2

Kinetics of phase separation in polymer solutions and blends. Structure of phase separated droplets. Size, shape, and distribution of micro domains measured using light and X-ray scattering, excimer fluorescence, time-resolved, small-angle X-ray scattering at the National Synchrotron Light Source. Studies of polymer-solvent systems, such as polystyrene-methylacetate, and polymer-polymer blends, such as polystyrene blended with polyvinyl methyl ether, polyisoprene, or polyorthochlorostyrene.

498. THEORETICAL STUDIES OF CHEMISORPTION AND SURFACE REACTIONS ON NICKEL AND SILICON

J. L. Whitten
Dept. of Chemistry
Phone: (516) 246-6068

$107,000 03-3

Theoretical studies of the adsorption of small molecules and molecular fragments on the surfaces of nickel and silicon using the embedding formulation of ab initio calculations. Energy contours and preferred surface adsorption sites are calculated along with vibrational frequencies for adsorbates. In some cases, excited electronic states will be calculated to help sort out the direct ionization vs. Auger processes that relate to electron or photon stimulated desorption from silicon surfaces. The embedding scheme is uniquely suited to these computations.

NORTH CAROLINA AGRICULTURAL AND TECHNICAL STATE UNIVERSITY
Greensboro, NC 27411

499. DEPOSITION OF AMORPHOUS SIC:H, AMORPHOUS SIO_2:H, AND TETRAHEDRAL-C THIN FILMS BY REMOTE PLASMA ENHANCED CVD AND PROGRAMMABLE IN SITU ETCHING

R. Tsu
Dept. of Electrical Engineering
Phone: (919) 334-7760

$ 80,000 01-5

Growth of thin film alloys of intrinsic, and n- and p-doped amorphous SiC:H, amorphous SiO_2:H and tetrahedral-c thin films by remote plasma enhanced chemical vapor deposition with programmable in-situ etching. Characterization using index of refraction, density measurements to be correlated with small-angle X-ray diffraction. Electrical and photoconductivity measurements.

NORTH CAROLINA CENTRAL UNIVERSITY
Durham, NC 27707

500. VIBRATIONAL PROPERTIES OF DISORDERED SOLIDS: FAR INFRARED STUDIES

J. M. Dutta
Dept. of Physics
Phone: (919) 683-6452
C. R. Jones
Dept. of Physics
Phone: (919) 683-6452

$ 30,000 02-2

Measurements of low-frequency vibrational properties of disordered solids in the far infrared region (5 cm^{-1} to 150 cm^{-1}) as a function of temperature using laser techniques. Materials studied: various forms of quartz and fused silica, alumina and magnesia. Other materials of interest: BeO, BN, and Si_3N_4. Effects on dielectric properties due to the presence and concentration of impurities and sintering acids, and to microstructural properties, investigated in selected materials. Experimental data compared with existing theoretical models.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27695

[redacted] THE STUDY OF STRUCTURE-PROCESSING-PROPERTY RELATIONS IN COPPER OXIDE-BASED HIGH T_c SUPERCONDUCTORS

A. I. Kingon
Dept. of Materials Science and Engineering
Phone: (919) 737-7907

$138,817 01-1

Investigate relationships between the crystallographic and electronic structure of copper oxide-based compounds and their electronic and superconducting properties. Fundamental understanding of the parameters determining the structure of the copper-oxygen sublattice. Study of aspects controlling grain boundary composition to provide structure-properties relationships.

502. FUNDAMENTAL ASPECTS OF EROSION AND IMPACT DAMAGE

R. O. Scattergood
Dept. of Materials Science and Engineering
Phone: (919) 737-7843

$139,187 01-5

Systematic study of fundamental aspects of erosion and impact damage in brittle materials and advanced ceramic systems. Materials investigated include aluminas, fiber-reinforced ceramics, transformation-toughened ceramics and various model brittle materials. New or modified apparatus designed and constructed for particle properties and threshold effects. Experimental results on erosion behavior and impact damage utilized for new fracture-mechanics analyses and erosion models development. Erosion rates vs. particle sizes, velocities and impact angles. Characterization of microstructural, strength and fracture properties. Erodent particle properties influence on nature of threshold effects.

NORTH CAROLINA STATE UNIVERSITY (continued)

503. RESEARCH AT AND OPERATION OF THE MATERIAL SCIENCE X-RAY ABSORPTION BEAMLINE (X-11) AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

D. E. Sayers
Dept. of Physics
Phone: (919) 737-2512

$325,000 (10 months) 02-2

Development and improvement of beamlines X-11 A and B at the National Synchrotron Light Source, Brookhaven National Laboratory. Installation of a focusing crystal system and a collimating mirror. Transmission, fluorescence and electron-yield measurements for a variety of materials and interfaces, including metal-metal, metal-semiconductor systems; multilayers and ion implanted layers; electrochemical systems; rare earth metal oxide catalysts; semiconductor alloys; high Tc superconductors; biocatalysts; and actinide metals. The materials, interfaces, and the specific properties to be examined in this investigation are important technical issues in materials science.

504. BAND ELECTRONIC STRUCTURES AND CRYSTAL PACKING FORCES

M. H. Whangbo
Department of Chemistry
Phone: (919) 737-3616

$ 91,739 03-1

Theoretical studies of superconducting and conducting, organic charge transfer salts. Tight-binding band electronic structure calculations on bis(ethylenedithio)tetrathiafulvalene (ET) salts using extended Huckel method. SCF-MO calculations on neutral and charged ET. Calculation of crystal packing energies, stabilities of different crystal phases, and magnitudes of electron-phonon coupling constants of various ET salts. Band structure calculations on high Tc superconductors.

UNIVERSITY OF NORTH CAROLINA
Chapel Hill, NC 27514

505. SOLID-STATE VOLTAMMETRY AND SENSORS IN GASES AND OTHER NON-IONIC MEDIA

R. W. Murray
Dept. of Chemistry
Phone: (919) 962-6295

$ 50,000 03-2

Preparation and electrochemical properties of systems in which a solid state polymer comprises the electrolyte between the electrodes. Observe electrochemical reactions in the absence of a liquid solution of electrolyte. The characteristics of electrocatalyzed reactions will be studied and the design of solid state sensors for gas phase measurements will be investigated.

NORTHEASTERN UNIVERSITY
Boston, MA 02115

506. POSITRON STUDIES OF DEFECTED METALS AND METALLIC SURFACES

A. Bansil
Dept. of Physics
Phone: (617) 437-2902

$ 89,500 02-3

Theoretical study with methods based on the Korringa-Kohn-Rostoker-coherent potential approximation of the momentum density in ordered compounds especially heavy-fermion systems (URu_2Si_2), high transition temperature superconducting ceramic compounds (La_2CuO_4), and high temperature superalloys (Ni_3Al). Disordered alloys, CuGe, and CuPd, and $Ni_{1-x}V_x$. Vacancy-type defects in metals and alloys. Surface related studies in metals and alloys. Metallic glasses (Ni-P and Fe-B). Compare with angular correlation of annihilation radiation (ACAR) experiments of electron-positron annihilation.

NORTHWESTERN UNIVERSITY
Evanston, IL 60208

507. ELECTRONIC AND STRUCTURAL PROPERTIES OF SEMICONDUCTOR HETEROJUNCTIONS

Y-W. Chung
Dept. of Materials Science and Engineering
Phone: (312) 491-3112

$ 46,623 01-1

Comprehensive investigation of α-Sn fibers deposited in UHV on single crystal CdTe substrate, including the study of the quantum size effect, using high-resolution electron energy loss spectroscopy and optical absorption; determination of the relationship between thermal degradation and interfacial diffusion in heterojunctions; determination of film growth characteristics using a site-specific xenon probe technique; and determination of structural and transformation characteristics using surface XRD at the NSLS, electron reflectivity techniques, and SIMS.

508. DEFECT CLUSTERING AND RELATED PROPERTIES OF OXIDES

J. B. Cohen
Dept. of Materials Science and Engineering
Phone: (312) 491-3665
D. E. Ellis
Dept. of Physics and Astronomy
Phone: (312) 491-3665
T. O. Mason
Dept. of Materials Science and Engineering
Phone: (312) 491-3198

$199,203 01-1

Study of defect clustering and related properties of oxides involving transport and nonstoichiometry measurements, diffraction, microscopy, and quantum theoretical methods. Oxides of interest include highly defective transition metal nonoxides (FeO, MnO, CoO, NiO), transition metal spinels (Fe_3O_4 and Mn_3O_4), stabilized ZrO_2, and ternary systems, e.g., $Ca_xNi_{1-x}O$ and high T_c superconductors. Transport and nonstoichiometry studies in a high oxygen potential cell at oxygen pressures of 1 to 100 atm. which permits substantially higher defect contents to be achieved. Structural and valence studies by X-ray and neutron diffraction, electron microscopy, and near edge absorption spectroscopy, utilizing select facilities at Argonne and Brookhaven National Laboratories. The theoretical program employs local density theory to calculate the charge distribution and local-site cohesion in defect oxides, describe phase stability (ternary oxides) and defect migration (stabilized zirconia), partly in conjunction with work at Argonne National Laboratory.

NORTHWESTERN UNIVERSITY (continued)

[redacted] NUCLEAR MAGNETIC RESONANCE CHARACTERIZATION OF POROUS STRUCTURES: CERAMICS AND SANDSTONES

W. P. Halperin
Dept. of Physics and Astronomy
Phone: (312) 491-3686

$ 92,000 01-1

Application of nuclear magnetic resonance measurements (spin-lattice relaxation and variable length scale diffusion) to determine topological information on the void space of ceramics and sandstones. Model materials including leached borosilicate (vycor) glasses and packings of monodisperse glass spheres. Investigations of fractal sandstones to define fractal dimensions. Results compared with those obtained on non-fractal sandstones in order to distinguish between dynamics in fractal and non-fractal geometries. Study of poor structure evolution during initial and intermediate sintering of alumina. Results used to refine sintering models and define relevant processing parameters. Study of magnetic grain alignment in high T_c superconductors.

510. CERAMIC SURFACES AND SINTERING

L. D. Marks
Dept. of Materials Science and Engineering
Phone: (312) 491-3996
D. L. Johnson
Dept. of Materials Science and Engineering
Phone: (312) 491-3996

$128,636 01-1

Atomistic investigation of ceramic particle sintering. High resolution phase contrast profile imaging of smoke particles agglomerated on gas columns for various times. Particle formation by vapor condensation and arc discharge in reactive gases. Chemical modifiers introduced by electrode and gas doping. Sintering experiments using Al_2O_3, oxide-free SiC, Si_3N_4, AlN and with selected ceramics modified by MgO, B and H_2O reactions. The atomic structure of particle surfaces and coalescent necks will be determined providing surface energy anisotropy, step distribution and chemical modifier information. Information to be input for atomistic model which will develop into a macroscopic continuum model.

NORTHWESTERN UNIVERSITY (continued)

511. MECHANISMS OF TRANSFORMATION TOUGHENING

G. B. Olson
Dept. of Materials Science and Engineering
Phone: (312) 491-2847

$220,444 01-2

Mechanisms of transformation toughening in ductile solids investigated by (a) detailed observations of crack-tip processes, and (b) numerical modeling with experimentally-derived constitutive relations. Model alloy steels (γ'-strengthened and phosphocarbide strengthened steels) used to study room temperature transformation toughening and constitutive behavior. Shear-instability-controlled fracture observed at sectional crack tips with and without transformation plasticity interactions using alloy composition to vary phase stability. Quantitative constitutive relations for experimental alloys applied to crack-tip and notch fields to study transformation plasticity interaction with various models of microvoid-softening-induced shear localization.

512. USE OF ANOMALOUS SMALL ANGLE X-RAY SCATTERING TO INVESTIGATE MICROSTRUCTURAL FEATURES IN COMPLEX ALLOYS

J. R. Weertman
Dept. of Materials Science and Engineering
Phone: (312) 491-5353

$100,793 01-2

An investigation is being carried out on the use of anomalous small angle X-ray scattering (ASAXS) to break down the scattering from a complex alloy into the components arising from each of the different scattering species, thereby making it possible to use the ASAXS data to obtain quantitative information about the size and number density of each species. Synchrotron radiation is used to provide X-rays which can be tuned to the absorption edge of elements in the alloy. ASAXS will be used to characterize the various scattering species in systems of interest and to study the changes in these scatterers produced by exposure to high temperature and deformation. The first system being studied is the ferritic stainless steel, modified Fe9Cr1Mo, which has already been examined by small angle neutron scattering. The value of ASAXS as a method of NDE will be investigated.

NORTHWESTERN UNIVERSITY (continued)

513. PLASMA, PHOTON, AND BEAM SYNTHESIS OF DIAMOND FILMS AND MULTILAYERED STRUCTURES

R. P. H. Chang
Dept. of Materials Sciences and Engineering
Phone: (312) 491-3598

$104,577 01-3

Investigation of the synthesis of high quality thick (micron to mm) films of diamond at substrate temperatures below 1000°C. Enhanced chemical vapor deposition experiments will invoke photon beams, charged particles, and magnetically confined plasmas. Analytical characterization of gas phase chemistry, surface reaction(s), and growth chemistry. Hetero-epitaxial growth of diamond films by a combination of growth techniques in an ultrahigh vacuum environment. Investigation of multilayered and superlattice structures of metallic to insulating and semiconducting diamond films. Mass spectroscopy, Auger spectroscopy, and RHEED analysis.

514. DEFECT STRUCTURE OF SEMICONDUCTING AND INSULATING OXIDES

B. W. Wessels
Dept. of Materials Science and Engineering
Phone: (312) 491-3537

$ 88,000 01-3

Characterization of defect structure including electrical compensation by deep level defects, thermal stability of native defects, and electrical and optical characterization of deep level defects in doped and electron and photon irradiated single crystal epitaxial oxide layers prepared by OMCVD. Comparison of theoretically predicted and experimentally determined deep level parameters. Experimental characterization of defect structure by photoluminescence and space charge spectroscopies. Materials of interest include ZnO, TiO_2, $SrTiO_3$, and other Ti based perovskites.

NORTHWESTERN UNIVERSITY (continued)

515. STRUCTURAL AND FAST ION TRANSPORT PROPERTIES OF GLASSY AND AMORPHOUS MATERIALS

D. H. Whitmore
Dept. of Materials Science and Engineering
Phone: (312) 491-3533
P. Georgopoulos
Dept. of Materials Science and Engineering
Phone: (312) 491-3243

$120,000 01-3

Detailed structural and ionic transport studies of fast ion conducting glasses including mixed valence, proton conducting and selenide based glasses and amorphous polyphosphazine polymer complexes. Investigation parameters include temperature, glass composition, and conditions of glass synthesis. Computer simulations of ionic transport in glassy electrolytes. Differential anomalous X-ray scattering, EXAFS, Raman and infrared spectroscopies, complex impedance analysis (of conductivity data) and pulsed field gradient NMR (to obtain ionic diffusivities). Mixed valence glasses synthesized by doping glass network formers with appropriate amounts of transition metal compounds investigated for the chemical diffusion coefficient, solid state redox reactions accompanying the insertion of electroactive alkali ion species into the mixed valence glass and the electronic transference number as a function of glass composition and temperature.

NORTHWESTERN UNIVERSITY (continued)

[redacted] ENERGETICS, BONDING MECHANISM AND ELECTRONIC STRUCTURE OF METAL/CERAMIC [redacted]

A. J. Freeman
Dept. of Physics and Astronomy
Phone No. (312) 491-3644

$ 43,913 02-3

Model the energetics, bonding, bonding mechanism and structure of metal/ceramic interfaces. Investigate surface electronic structure of oxides and the simple interface grain boundaries in transition metal-simple oxide interfaces, e.g., MgO and NiO; metals interfaced with covalently bonded ceramics such as SiC; Pd-Al_2O_3 and spinel-metal interfaces, e.g., Ag/$MgAl_2O_4$; and metal/high Tc superconductor systems. Determine the role of interfacial impurities, such as the irreversible trapping of hydrogen.

517. [redacted] ELECTROCHEMICAL TRANSPORT IN BATTERIES

M. A. Ratner
Dept. of Chemistry
Phone: (312) 491-5655
D. F. Shriver
Dept. of Chemistry
Phone: (312) 491-5655

$ 93,000 03-2

This proposal is an investigation of ionic transport along and through interfaces, both within a given solid electrode or electrolyte and between solid electrodes and electrolytes. The objective is mechanistic understanding of which processes result in overpotential, degradation, charge accumulation, and enhanced mobility at such interfaces. Two general classes of materials will be investigated: siloxane based polymer electrolytes, and layered chalcogenide cathodes. Experiments will include synthesis and surface modification of electrolyte films, bulk and interfacial impedance measurements, and simulation of interfacial transport phenomena by Monte Carlo and percolation theory techniques.

NORTHWESTERN UNIVERSITY (continued)

518. STUDIES OF THE STRUCTURE AND PROPERTIES OF ORGANIC MONOLAYERS, MULTILAYERS AND SUPERLATTICES

P. Dutta
Dept. of Physics and Astronomy
Phone: (312) 491-5465
J. B. Ketterson
Dept. of Physics and Astronomy
Phone: (312) 491-5468

$305,805 03-3

Study the mechanical properties of organic monolayers on the surface of water (Langmuir films). Determine the microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) using ellipsometry, conventional and synchrotron X-rays. Mechanical property studies directed toward shear response, an important but previously neglected structural property. Diffraction technique, involving external reflection at the monolayer surface, used to determine film structure. Finally, the loss of certain symmetry elements of surface phases studied by observing the rotation of plane polarized light incident normal to the surface. A search for this effect within the so-called liquid expanded-liquid condensed region, may indicate a liquid crystal phase.

NOTRE DAME, UNIVERSITY OF
Notre Dame, IN 46556

519. SINGLE-ELECTRON CHARGING EFFECTS

S. T. Ruggiero
Department of Physics
Phone: (219) 239-7463

$ 36,000 02-2

The electrical characteristics (e.g., current-voltage) of ultra-small capacitance systems will be studied. The principal investigator has already observed single-electron charging effects in tunnel junctions containing ensembles of small Ag particles. Investigations of junctions containing superconducting and magnetic particles are planned. Also planned are experiments in which the electrical characteristics are changed by the introduction of microwave radiation. The experiments explore the electronic properties of metallic particles 10-100 A in diameter.

OHIO STATE UNIVERSITY
Columbus, OH 43210

521. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT [redacted] SEPARATING ANISOTROPIC MATERIALS

L. Adler
Dept. of Welding Engineering
Phone: (614) 292-1974

$140,255 01-5

Fundamental research program on non-destructive characterization of polycrystalline anisotropic materials. Specific activities will include modeling and measurement of ultrasonic wave propagation in Ni bicrystals, treatment of the effects of structural imperfections at grain boundaries on ultrasonic characterization, and experimental studies using scanning acoustic microscopy.

[redacted] THE HYDROGEN-INDUCED STRESS CORROSION CRACKING OF NICKEL BASE ALLOYS IN HIGH TEMPERATURE WATER

P. G. Shewmon
Dept. of Metallurgical Engineering
Phone: (614) 292-5864
S. Smialowska
Dept. of Metallurgical Engineering
Phone: (614) 292-0290

$151,686 01-5

Research on the mechanism of the hydrogen induced intergranular stress corrosion cracking (IGSCC) of Alloy 600, of austenitic Cr-Ni steels, and of other Ni-containing alloys on exposure to deaerated water at 300-363^{o}C. Determination of the electrochemical conditions under which hydrogen induced IGSCC occurs in materials of different composition and microstructure. Determine crack growth rates as a function of environmental parameters such as electrolyte composition, pH, electrochemical potential, temperature and partial pressure of hydrogen. Examine the composition and protective properties of oxide films that form on fcc nickel-base alloys under various environmental conditions and evaluate the effect of those films on IGSCC and hydrogen absorption. Study the micromechanism of fracture with emphasis on the possible role of grain boundary bubbles of methane.

OHIO STATE UNIVERSITY (continued)

522. THEORETICAL STUDIES OF DYNAMICS AND CORRELATIONS IN HEAVY-ELECTRON MATERIALS

D. Cox
Dept. of Physics
Phone: (614) 292-0620

$ 52,471 02-3

Examine the universality of the Anderson model for heavy-electron metals, specifically a form of the Anderson impurity model for a single U impurity, and analysis of magnetic susceptibility of UBe_{13} in terms of a quadrupolar Kondo effect. Study coherence and the transport properties of the Anderson lattice; a model for transport properties that predicts ac and dc conductivities and tunneling and point contact spectra in Ce compounds. Understanding intersite correlations between f-electrons and the relation to magnetic ordering and heavy fermion superconductivity.

523. STRONGLY INTERACTING FERMION SYSTEMS

J. W. Wilkins
Department of Physics
Phone: (614) 292-5713

$ 75,000 02-3

Theory of heavy fermion behavior in lanthanide and actinide compounds, and more generally of systems with f and/or d electrons that are strongly interacting or correlated and of superconductors with high critical temperatures. Aims at understanding the occurrence or absence of heavy fermions in such systems, the nature of the low temperature coherent state, the transition to a Kondo-like state at higher temperatures, and an account of the unusual magnetic and superconducting properties of the materials. Both the one and two impurity Anderson models are studied, the former within the framework of the self-consistent large N expansion approach, and the latter using a numerical renormalization group approach. A new study of high-Tc materials has begun with an emphasis on understanding the ground state of the two-dimensional Hubbard model and the effects of Coulomb correlations on the electronic band structure.

OHIO STATE UNIVERSITY (continued)

524. MOLECULAR FERROMAGNETISM

A. J. Epstein
Dept. of Physics
Phone: (614) 292-1133
J. S. Miller
E. I. duPont de Nemours & Co.
Central Research & Development Dept.
Experimental Station
Wilmington, DE 19898
Phone: (302) 695-1199

$174,900 03-1

Study of magnetism in molecular ferromagnets and origins of the ferromagnetic exchange. Synthesis of $[M(C_5(CH_3)_5)_2]^+$ and $[M(C_6R_6]^+$ (M=Cr, Fe, Ru, and Ni) salts of planar radical anions 7, 7, 8, 8-tetracyano-pquinodimethane (TCNQ), tetracyanoethlene (TCNE), and 2, 3-dichloro-5, 6-dicyanobenzoquinone (DDQ). Measurements of magnetism as a function of field, temperature, and pressure and comparison of results with models of one-dimensional ferroferrimagnetism. Mossbauer spectroscopy measurements for internal magnetic fields, spectroscopic measurements for charge transfer bands and inelastic neutron scattering measurements for magnetic structure.

OHIO UNIVERSITY
Athens, OH 45701

525. ELECTRONIC STATES IN TUNNELING SEMICONDUCTOR SUPERLATTICES

S. E. Ulloa
Dept. of Physics and Astronomy
Phone: (614) 593-1729

$ 99,910 (24 months) 02-3

Theory of semiconductor interfaces, specifically the electronic states in doped semiconductor superlattices which allow tunneling along the direction of modulated growth, perpendicular to the composing layers. Work includes self-consistent calculations of the electronic structure and the resulting effects on transport properties of levels associated with depletion regions near the top and bottom layers of superlattices. These defect- and impurity-associated levels will have important implications for a variety of other experimental arrangements. It may be possible to use the physical responses to external perturbations as a novel and potentially powerful tool in the detailed experimental mapping of the electronic level structures of these systems.

OKLAHOMA STATE UNIVERSITY
Stillwater, OK 74078

526. RHEO-OPTICAL STUDIES OF MODEL "HARD SPHERE" SUSPENSIONS

B. J. Ackerson
Dept. of Physics
Phone: (405) 624-5819

$110,000 01-3

Colloidal suspensions undergoing steady linear shear flow and large amplitude oscillatory shear flow studied using light scattering and rheological measurements. Uniformly sized spheres suspended in solvent to match particle index of refraction. Range of shear parameters and particle concentrations investigated and results compared to theory. Inducement of large scale "single" crystal order by special shear flow processing.

527. RADIATION DAMAGE OF TRANSITION METAL CARBIDES

C. Y. Allison
Dept. of Physics
Phone: (405) 624-5811

$ 85,675 01-4

Investigation of effects of neutron and electron irradiation on transition metal carbides of groups IV and V. Particular emphasis on the effects of irradiation on the ordered carbon vacancy phases which result from nonstoichiometry. Radiation damage studied by electrical resistivity, Hall effect, optical properties and electron microscopy. Ultimate objective to understand effects of radiation damage on point defects and ordered phases in these materials.

OREGON STATE UNIVERSITY
Corvallis, OR 97331

[redacted] HYPERFINE EXPERIMENTAL INVESTIGATION OF ZIRCONIA CERAMICS

J. A. Gardner
Dept. of Physics
Phone: (503) 754-4631

$110,000 01-1

Perturbed angular correlation (PAC) spectroscopy of nuclear gamma rays to investigate Zr-containing ceramics. PAC characterization of free energies, transformation mechanisms, equilibrium phase boundaries, diffusion and relaxation models, short range order, order-disorder reactions, and elevated temperature time dependent effects in various zirconia's that are prepared to typically contain ^{181}Hf or ^{111}In as a probe. Investigation of ^{91}Zr in zirconia by nuclear quadrupole resonance (NQR) and of ^{17}O substituted zirconia by nuclear magnetic resonance (NMR). NMR/NQR experiments to complement and expand the local structure and oxygen vacancy dynamics studies underway with PAC.

529. THEORETICAL STUDIES OF ZIRCONIA AND RELATED MATERIALS

H. J. F. Jansen
Dept. of Physics
Phone: (503) 754-4631

$ 85,392 01-3

Total energy calculations of the electronic structure of zirconia and related materials used to obtain the electronic energy and the charge density as a function of atomic arrangement. Study of field-gradients, lattice relaxation, phonon spectrum, oxygen mobility and transport. Both Full Potential Linearized Augmented Plane Wave (FLAPW) and Monte Carlo techniques used.

UNIVERSITY OF OREGON
Eugene, OR 97403

530. SURFACE AND [redacted]CE ELECTRONIC STRUCTURE

S. D. Kevan
Dept. of Physics
Phone: (503) 686-4742

$150,000 02-2

An experimental investigation of the electronic structure of surfaces and interfaces including studies of angle-resolved photoemission at the National Synchrotron Light Source. Emphasis on high resolution studies of novel surface phenomena such as phase transitions, small perturbations of the ground state electronic structure by defects and impurities, and initial stages of epitaxial interface formation between metals and semiconductors.

531. MONITORING [redacted] DYNAMICS BY PULSED LASER TECHNIQUES

G. L. Richmond
Dept. of Chemistry
Phone: (503) 686-4635

$ 99,578 03-2

Studies of interfacial structure and dynamics using second harmonic generation (SHG) and hyper-Raman scattering. Development of SHG for monitoring electrochemical reactions on a nanosecond time scale, correlation of surface structure with electron transfer kinetics, thin-film nucleation and growth, and the analyses of the structure and reactive role of surface defects.

PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

532. VIBRATIONAL AND OPTICAL STUDIES OF AMORPHOUS METALS

J. S. Lannin
Dept. of Physics
Phone: (814) 865-9231

$124,894 01-1

Research in which the method of interference-enhanced Raman scattering (IERS) is used to study the structure, bonding, and stability of amorphous metal alloys. The basis of the IERS technique is to fabricate thin film trilayer structures of the materials to be studied which include a dielectric layer and a reflecting layer to produce a minimum in the reflectance and thus reduce the background light when measuring the Raman scattered light. Focus is initially on metalloid alloys and will subsequently be extended to amorphous metals in general. Complementary inelastic neutron scattering measurements are also employed for structure, bonding, and short-range order determinations.

533. THE MECHANICAL BEHAVIOR OF SURFACE MODIFIED CERAMICS

D. J. Green
Dept. of Materials Science and Engineering
Phone: (814) 863-2011

$ 85,946 01-2

Modification of surface layers of ceramics to introduce surface compression and increase hardness and fracture toughness of transformation toughened ZrO_2 and Al_2O_3. Surface infiltration when ceramic is pressed or partially sintered. Development of a second phase surface layer during final densification. Indentation cracking used to study crack nucleation and growth and determine fracture toughness. Stress and composition profiles determined by NSLS X-ray diffraction data.

PENNSYLVANIA STATE UNIVERSITY (continued)

534. [redacted]ND MODULATED STRUCTURES IN MARTENSITES

G. R. Barsch
Materials Research Laboratory
Phone: (814) 865-1657

$150,000 01-3

Theoretical study with concurrent supporting experimental investigations on coherent and semicoherent interfaces in ferroelastic martensites, including twin boundaries and twin bands, interfaces, modulated structures, and transformation precursors. Motivation is the need for a new theoretical basis for investigating the martensite nucleation mechanism and for establishing the conditions for nonclassical nucleation. Study of soliton-like solutions of a dynamic Ginzburg-Landau continuum theory for ferroelastic martensites in order to determine the strain distribution and strain energy for various geometric configurations as a function of the material parameters, temperature and external stress. Model parameters of the theory consist of the second and higher order elastic constants and the harmonic strain gradient coefficients in the parent phase. Elastic and inelastic neutron scattering and X-ray measurements of the transformation strain versus temperature. Simultaneous ultrasonic velocity and attenuation measurements on biaxially stressed crystals in $In_{1-x}Tl_x$ alloys in order to determine the second and higher order elastic constants in the single domain tetragonal state. Special attention is given to transformation precursors in the cubic parent phase in order to eliminate their effect on the model parameters.

535. [redacted]Y AND SURFACE DIFFUSION IN [redacted]

V. S. Stubican
Dept. of Materials Science and Engineering
Phone: (814) 865-9921

$ 46,732 01-3

Research addresses surface diffusion on ionic surfaces. In particular, the diffusion of Co on the surfaces of NiO and Fe_3O_4 will be studied and the influence of the point defect structure determined.

PENNSYLVANIA STATE UNIVERSITY (continued)

536. MASS TRANSFER DURING LASER WELDING

T. DebRoy
Dept. of Materials Science and Engineering
Phone: (814) 865-1974

$ 81,503 01-5

Modeling of solute loss, heat transfer and fluid flow during laser welding of stainless steels. Calculation of local temperature profile, weld pool velocity and vaporization of alloying elements; correlative experimental determination of weld microstructure and chemistry; time resolved emission spectroscopic measurements to determine composition of metal vapors.

537. TOPOTACTIC AND EPITACTIC ROUTES TO NEW MATERIALS

R. Roy
Materials Research Laboratory
Phone: (814) 865-3421

$ 82,708 03-2

Synthesis and characterization of crystalline materials formed at low temperatures. The objective is to apply some of the very new and exciting advances in chemically-bonded ceramics to making much stronger and more impermeable materials that can be processed at low temperatures. The material has potential application as low-level radioactive waste hosts.

UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

538. STAGING IN LAYER INTERCALATES

J. E. Fischer
Dept. of Materials Science and Engineering
Phone: (215) 898-6924

$134,121 01-1

Study of the staging phenomenon in graphite intercalation compounds (principally with Li) and other layer systems by X-ray and neutron diffraction. Independent variables are temperature, hydrostatic pressure and concentration of alkali metal intercalate. Experimental determination of the staging temperature vs. concentration phase diagram. Elucidation of new high-pressure phases. Determination of the nature, origin, and consequences of stage disorder. Investigation of kinetics of staging transitions with emphasis on identifying metastable structures.

UNIVERSITY OF PENNSYLVANIA (continued)

539. ATOMISTIC STUDIES OF GRAIN BOUNDARIES IN ALLOYS AND COMPOUNDS

V. Vitek
Dept. of Materials Science and Engineering
Phone: (215) 898-7883

$141,476 01-1

Atomistic computer simulation studies of grain boundaries in binary ordered and disordered alloys. Investigation of grain boundaries with segregated solutes. Examination of the relationship between grain boundary structure and surfaces formed by fracturing along these boundaries. Study of grain boundary electronic structure. Methods of calculation of interatomic forces. Cu-Bi, Cu-Ag, Ag-Au, Ni-S, Fe-P, Fe-Sb, and Fe-Sn are candidate alloys to be studied.

540. LOW STRESS BRITTLE FRACTURE IN POLYMERS

N. Brown
Dept. of Materials Science and Engineering
Phone: (215) 898-8506

$ 91,782 01-2

Research on polyethylene, copolymers and representative crystalline polymers. Measurement under plane strain of rate of formation of damaged zone at root of a notch as a function of stress, time, temperature, notch depth, specimen geometry. Characterization of extent of porous, fibrillated and fractured regions which constitute the damaged zone using optical microscopy, SEM, and TEM. Determination of constitutive equations for various regions of damaged zone. Use of data to construct a mathematical model based on the micro-mechanics of fracture for predicting long time failure in engineering structures.

UNIVERSITY OF PENNSYLVANIA (continued)

541. FUNDAMENTALS OF HARDENING AND DECOHESION BEHAVIOR IN TIME-DEPENDENT CYCLIC DEFORMATION

C. Laird
Dept. of Materials Science and Engineering
Phone: (215) 898-6664
J. L. Bassani
Dept. of Mechanical Engineering and Applied Mechanics
Phone: (215) 898-5632

$189,192 01-2

Investigation of latent hardening and strain localization in single crystals under cyclic deformation and modeling of polycrystalline cyclic stress-strain behavior to understand the conditions under which strain localization and, particularly, the plateau in the cyclic stress-strain curve occurs. Results obtained on cyclically deformed single crystals of various orientations used to develop quantitative laws to predict the behavior of polycrystalline materials. Predictions compared to experimental results. Fundamental understanding of latent hardening and strain localization; manifestations of plastic flow concentrations such as persistent slip bands which appear under cyclic loading.

[redacted] MECHANISMS OF DIFFUSION CONTROLLED BRITTLE FRACTURE

C. J. McMahon
Dept. of Materials Science and Engineering
Phone: (215) 898-7979

$105,527 01-2

Study of the mechanisms of diffusion-controlled intergranular brittle fracture of metallic materials due to surface-adsorbed impurities. Measurement of the kinetics of intergranular crack growth in polycrystals and bicrystals with controlled surface coverages of impurities, carried out in UHV. Major experimental variables are: impurity coverage, temperature, alloy strength, and applied stress or loading rate. Measurements of the plastic behavior of the alloy, surface and grain boundary diffusion rates, and grain boundary/surface dihedral angles will be used to test models proposed to explain this phenomenon.

UNIVERSITY OF PENNSYLVANIA (continued)

543. STRUCTURE AND VIBRATIONAL EXCITATIONS OF RECONSTRUCTED SEMICONDUCTOR SURFACES

E. J. Mele
Dept. of Physics
Phone: (215) 898-7293

$ 57,000 02-3

Theoretical studies of the lattice dynamics of reconstructed semiconductor surfaces. Relation between localized surface electronic structure and surface structural and vibrational properties. Computations, employing developed theoretical model, will investigate the surface vibration excitations of elemental group IV semiconductors. Application of model to study the self trapping of extrinsic charges on clean low index surfaces of Si. Analysis of the low lying vibrational degrees of freedom in the Takayanagi model for Si (111) 7x7, extensions to higher order reconstructions. Application of theory to 2x1 phase of the Ge(111) surface and the 2x2 surface of C(111).

UNIVERSITY OF PITTSBURGH
Pittsburgh, PA 15261

[redacted] MICROCHEMISTRY ANALYSIS OF INTERMETALLIC ALLOYS USING THE FIELD-ION MICROSCOPE ATOM PROBE

S. S. Brenner
Dept. of Materials Science and Engineering
Phone: (412) 624-9738

$145,256 01-1

Investigation of structure and microchemistry of grain boundaries in Ni_3Al containing different Ni/Al stoichiometric ratios, substitutional solutes, and grain boundary B concentrations. Studies to be extended to NiAl, Ni_3Si, Co_3Ti, Ni_3Ga and Ni_3Mn. Principal analytical methods involve the field-ion microscope atom probe. Other variable parameters include grain-boundary orientation, bulk B concentration, Al substoichiometry, and comparison between cast and melt-spun materials.

UNIVERSITY OF PITTSBURGH (continued)

[redacted] THE PHYSICS OF PATTERN FORMATION AT LIQUID [redacted]

J. V. Maher
Dept. of Physics and Astronomy
Phone: (412) 624-9007

$130,766 02-2

Experimental investigation of non-equilbrium phenomena at liquid interfaces. Viscous fingering in rectangular and circular Hele-Shaw cells. Variations of initial conditions to determine transient flow patterns. Staffman-Taylor instability. Comparison of fingering flows in open and closed cells. Role of interfacial tension. Fingering in a non-Newtonian liquid. Flows at low and high velocity. Binary liquid gels and polymer solutions. Establish connections between these systems and other recent work on pattern formation, nonlinear growth, and transition to turbulence.

POLYTECHNIC UNIVERSITY
333 Jay Street
Brooklyn, NY 11201

546. SCANNING TUNNELING MICROSPECTROSCOPY OF SOLIDS AND SURFACES

E. Wolf
Dept. of Physics
Phone: (718) 643-2070

$133,000 02-2

Development of Scanning Tunneling Microscopy (STM) techniques as applied to the study of solids and surfaces. Probe both normal and superconducting states of materials. Basic information about the new class of many-body states in heavy fermion materials. Pairing symmetry study of $La_{1.8}Sr_{0.2}CuO_4$ a new high temperature superconductor. Basic superconducting tunneling phenomena; Josephson and proximity effects. Importance of spin-orbit coupling arising from the f electron character of the heavy quasiparticles in heavy fermion materials. Quasiparticle spectroscopy of exotic conductors including organic superconductors.

POLYTECHNIC UNIVERSITY (continued)

547. HEAVY FERMION AND ACTINIDE MATERIALS

P. S. Riseborough
Dept. of Physics
Phone: (718) 643-5011

$ 63,379 02-3

Study the properties of the Anderson lattice in a manner which does not require the assumption of either the presence of specific f-electron configurations in the ground state wave functions or of a Hubbard splitting between excited f-electron configurations containing one more or less electron per atom. The absence of these assumptions makes the treatment more applicable to the study of uranium systems. Specifically, single particle excitation spectra are calculated for comparison with photoemission and Bremstrallung isochromatic spectra, as well as the effects of spin dynamics on inelastic neutron scattering, NMR, magnetic susceptibility and ESR of uranium materials and heavy electron superconductors. Comparison of coupling mechanisms in heavy electron superconductivity and those possible in the new high T_c superconducting oxides.

PRINCETON UNIVERSITY
Princeton, NJ 08544

548. CONTROL OF MICROSTRUCTURE DURING CONSOLIDATION AND INJECTION MOLDING OF COLLOIDAL DISPERSIONS

W. B. Russel
Dept. of Chemical Engineering
Phone: (609) 452-4590

$ 89,430 01-3

The dynamics of three processes (sedimentation, ultrafiltration, and slip casting) which concentrate small particles from a dilute solution, with particular emphasis on the structure of the resulting dense phase as a function of the processing conditions. Objectives are to define the range of conditions which produce an ordered casting, develop process models, and perform measurements of diffusion models in dense suspensions. Modeling to involve the formulation and solution of a macroscopic conservation equation governing the mean volume fraction, coupled to a microstructural equation describing the relaxation of imperfections enroute to the equilibrium ordered state. Dynamic light scattering experiments on concentrated silica dispersions to determine diffusion coefficients. Sedimentation and ultrafiltration experiments following the formation of both disordered and ordered phases.

PRINCETON UNIVERSITY (continued)

549. ASPECTS OF PHOTOIONIZATION OF IMPURITIES AND ELECTRON TRANSFER IN IONIC CRYSTALS

D. S. McClure
Dept. of Chemistry
Phone: (609) 452-4980

$109,751 03-1

Research on the mechanisms by which impurity ions in host ionic crystals lose an electron when photo-excited. A newly developed tunable infrared laser is used in two-photon pump-probe type experiments to determine how the impurity ion and host lattice change as the photoelectron is lost or regained. Phototransfer of electrons from one impurity ion to another is studied as a function of separation in the host lattice. New compounds are synthesized with the impurity ion in an octahedral rather than cubic environment, which should raise the photoemission threshold. New lasing media tunable in the VUV are a possibility.

PURDUE UNIVERSITY
West Lafayette, IN 47907

550. THE ROLE OF MOBILE IONS IN FAST ION CONDUCTING SYSTEMS AND HIGH-IMPACT CERAMICS

C. A. Angell
Dept. of Chemistry
Phone: (317) 494-5256

$ 94,387 01-1

Seek novel materials exhibiting fast ion transport and high rates of energy dissipation on impact. Anionic conductivities in lead-halide-rich inorganic glasses, mixed anion-cation conducting glasses, mixed ionic-electronic conductivity tellurovanadate glasses with high Na^+ transport and new organic cation containing plastic crystal conductors. Objectives are clarification of mobile cation-anion coupling in conducting glasses, exploitation of Na^+ transport in an oxygen-fugacity-controlled electronic oxide conducting glass, development and optimization of rotator phase ionic conductors. Secondarily, explore possibility that fast processes can provide fast energy dissipation and utilize computer simulation calculations to study fast processes by dynamic graphics methods.

PURDUE UNIVERSITY (continued)

551. MATERIALS RESEARCH AND BEAM LINE OPERATION UTILIZING NSLS

G. L. Liedl
School of Materials Engineering
Phone: (317) 494-4095

$400,000 01-1

A grant to support MATRIX, a group of scientists from several institutions who have common interests in upgrading and in utilizing X-ray synchrotron radiation for unique materials research. The group has available a specialized beam line at the National Synchrotron Light Source (NSLS). A unique and versatile monochromator provides radiation to a four-circle Huber diffractometer for the basic system. Multiple counting systems are available as well as a low temperature stage, a high temperature stage, and a specialized surface diffraction chamber. The grant covers the operational expenses and system upgrade of this beam line at NSLS for all MATRIX members and to support part of the research on phase transformation studies, and X-ray surface and interface studies.

[redacted] STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA

H. Sato
School of Materials Engineering
Phone: (317) 494-4099
R. Kikuchi
School of Materials Engineering
Phone: (317) 494-4099

$114,330 01-3

Research on multicomponent diffusion under general thermodynamical potential gradients. Chemical diffusion processes in alloys--diffusion path, zero flux planes, and Kirkendall effect--analytically based on an atomistic model. Investigation of diffusion paths through a different phase between diffusion couples and in demixing profiles. Interdiffusion at boundaries. Interdiffusion in artificial superlattices in semiconductors. Continued examination of demixing phenomena.

PURDUE UNIVERSITY (continued)

[redacted] GAMMA SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION

J. G. Mullen
Dept. of Physics
Phone: (317) 494-3031

$ 62,885 02-2

Development of new Mossbauer techniques with a microfoil electron detector, LiF monochromator, and high intensity sources. Accurate measurement of the Mossbauer isomer for the 46.5 keV transition in ^{183}W. Test of time reversal invariance in gamma emission accompanying nuclear decay to an order of magnitude greater accuracy than previously attained. Resonance scattering from TaS_2-1T that permits study of the charge density wave phenomena in this material. Thermal diffuse scattering and Debye-Waller factor scattering between temperatures of 77 and 295 Kelvin (room temperature). Attempted measurement of inelastic scattering, resulting from one phonon processes near the edge of the Brillouin zone.

554. A STUDY OF THE INTERACTION OF LIGHT WITH SURFACES OF SUB-MICRON DIMENSIONS

R. G. Reifenberger
Dept. of Physics.
Phone: (317) 494-3032

$ 65,500 02-2

Investigation of the photoexcitation process at low photon energies. Techniques under development directly measure the excited state energy distribution of electrons that are emitted through the surface potential barrier. The fundamental process; photoexcitation of electrons from field emission tips by a focussed argon-ion laser beam tuned to operate at a specific photon energy. Measurement of localized surface states on semiconducting and carbide materials. Laser-induced diffusion and desorption effects associated with illumination of adsorbate-covered, sub-micron surfaces. Exploration of advantages and properties of a laser-illuminated scanning tunneling microscope.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, NY 12181

555. MECHANISM OF MECHANICAL FATIGUE IN FUSED SILICA

M. Tomozawa
Dept. of Materials Engineering
Phone: (518) 276-6451

$110,000 01-2

Mechanism of cyclic fatigue and analysis of fatigue kinetics in fused silica. Measurement of diffusion coefficient and solubility of water in silica glass as a function of stress, temperature and water vapor pressure. Preparation of silica glass containing various water contents. Effect of water content on swelling and mechanical property alteration. Effect of environment on crack initiation and propagation. Comparison of cyclic and static fatigue in various environments.

556. STABILIZATION OF HIGH T_C SUPERCONDUCTIVITY IN CdS

R. K. MacCrone
Dept. of Materials Engineering
Phone: (518) 276-6047

$177,024 01-3

Precise chlorine doping used to ameliorate irreproducibility and/or instability in measurements indicating superconductivity in CdS. Material will be subjected to pressure quenching and thermal treatments and tested for superconductivity. Structural state of the material will be characterized by ion chromatography, X-ray diffraction, photo-acoustic spectroscopy and EPR.

RICE UNIVERSITY
P. O. Box 1892
Houston, TX 77251

557. APPLICATION OF SPIN-SENSITIVE ELECTRON SPECTROSCOPIES TO INVESTIGATIONS OF ELECTRONIC AND MAGNETIC PROPERTIES OF SOLID SURFACES AND EPITAXIAL SYSTEMS

G. K. Walters
Physics Dept.
Phone: (713) 527-4937
F. B. Dunning
Dept. of Physics
Phone: (713) 527-8101

$235,520 02-4

Spin polarized beams of electrons and metastable He(2^3S) atoms used in studies of surface magnetic behavior, dynamics of metastable deexcitation at surfaces, electronic properties of adsorbed layers. Spin Polarized Low Energy Electron Diffraction (SPLEED) and Metastable Deexcitation Spectroscopy (MDS) investigations of magnetic properties of epitaxial systems at the monolayer level. Emphasis on monolayers of Cr on Au(110), and monolayers of V and Fe on Ag(001) for which theory predicts strongly enhanced two-dimensional ferromagnetic moments on metallic overlayers, interfaces, and superlattices.

UNIVERSITY OF ROCHESTER
Rochester, NY 14623

558. MICROSTRUCTURAL BEHAVIOR OF NON-EQUILIBRIUM SYSTEMS

J. C. M. Li
Dept. of Mechanical Engineering
Phone: (716) 275-4038

$132,100 01-2

Coupled theoretical and experimental research on amorphous metals. Topics include: a) negative creep of amorphous metals studied from the viewpoint of a mechanical spinodal and its properties, b) molecular dynamics simulation of melting, c) dislocations in amorphous metals as detected by magnetic domain patterns, d) dislocations emitted from a Mode I crack, (e) effect of grain size on fracture toughness, and f) processing of high T_C superconducting ceramics.

UNIVERSITY OF ROCHESTER (continued)

559. DYNAMICS OF SURFACE MELTING

Hani E. Elsayed-Ali
Lab. for Laser Energetics
Phone: (716) 275-5101

$163,270 (16 months) 03-3

Experimental study of the melting transition of metal single crystals focusing on the occurrence and nature of surface melting. Picosecond time resolved reflection high energy electron diffraction (RHEED) will be used as a surface structure probe. The fast time resolution will be used to examine the dynamical processes taking place during the melting transition. Picosecond laser heating will be employed. Initially, low index facets of lead, bismuth, zinc and cadmium will be examined.

ROCKWELL INTERNATIONAL SCIENCE CENTER
1049 Camino Dos Rios/Box 1085
Thousand Oaks, CA 91360

560. ADVANCED Si_3N_4 SYSTEM STUDIES

P. E. D. Morgan
Phone: (805) 373-4273

$157,985 01-5

Investigations of Si-S chemistry to provide starting points for the preparation of Si_3N_4 and SiC in various forms such as powder, whiskers, fibers, etc. Room temperature reactions of SiS_2 with hydrazine. TGA, XRD, TEM, NMR, IR, fracture toughness.

RUTGERS - THE STATE UNIVERSITY
Piscataway, NJ 08854

561. MULTICOMPONENT GLASS SURFACES: STRUCTURE AND ADSORPTION

S. H. Garofalini
Dept. of Ceramics
Phone: (201) 932-2216

$150,000 01-3

Surface structure of multicomponent silicate glasses and the effect of structure on adsorption behavior. Molecular dynamics computer simulations of surfaces and surface behavior. Surface analysis to study adsorbate-substrate systems of the type considered in the simulations. Applications of ISS, SIMS, AES, and XPS to surface adsorption phenomena.

SETON HALL UNIVERSITY
South Orange, NJ 07079

562. SYSTEMATIC PREPARATION OF SELECTIVE HETEROGENEOUS CATALYSTS

R. L. Augustine
Dept. of Chemistry
Phone: (201) 761-9033

$ 75,000 03-3

Apply previously developed single-turnover titration method for characterizing the active site distribution on metal surfaces to supported metal catalysts such as Pt/Al_2O_3, Pt/SiO_2, and Pt/TiO_2. Examine change in site distribution with method of preparation, metal particle size, and type of support. Modify the site distribution with chiral ligands such as phosphines, sulfides and/or carbonyls. Optimize chiral modifiers to produce highly selective hydrocarbon catalysis.

SOUTHWEST RESEARCH INSTITUTE
6220 Culebra Road
San Antonio, TX 78284

[redacted] CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION

R. A. Page
Dept. of Materials Science
Phone: (515) 522-3252
J. Lankford
Dept. of Materials Science
Phone: (515) 522-2317

$168,053 01-2

Characterization of pore evolution during sintering and cavitation during creep. Objectives of the sintering study are the statistical characterization of pore evolution during densification, identification of primary variables affecting pore removal, and development and evaluation of sintering models. Objectives of the creep study are to understand the effects of microstructural parameters and loading mode including uniaxial tension on the kinetics of various creep mechanisms such as grain boundary sliding and cavity growth. Small angle neutron scattering (SANS) measurements supplemented by TEM, SEM, precision density and AES characterization, tensile-creep measurements, and grain boundary sliding measurements by a stereo-imaging technique. SANS measurements at the 30m instrument at the National Center for Small-Angle Scattering Research at ORNL and the 8m instrument that is being upgraded with a cold source at NBS. Cavity size, distribution, morphology, and nucleation and growth rates determined by SANS analysis. Principal experimental materials: Al_2O_3 and SiC.

SRI INTERNATIONAL
Menlo Park, CA 94025

564. FUNDAMENTAL STUDIES ON PASSIVITY AND PASSIVITY BREAKDOWN

D. D. Macdonald
Chemistry and Chemical Laboratories
Phone: (415) 859-3195

$208,086 01-3

Development of a comprehensive physical model for the phenomenon of passivity breakdown. Theoretical and experimental studies of effects of minor alloying elements on passivity breakdown. Models for the distributions in breakdown parameters. Physics and electrochemistry of photo-inhibition of passivity breakdown. Alloy specimens formed by ion implantation. Experimental techniques include time-elapsed optical microscopy, low frequency AC impedance spectroscopy, and photo-electrochemical impedance spectroscopy.

STANFORD UNIVERSITY
Stanford, CA 94305

565. INTERNAL-VARIABLE BASED MODELS FOR ELEVATED-TEMPERATURE FATIGUE AND DEFORMATION

A. K. Miller
Dept. of Materials Science and Engineering
Phone: (415) 723-3732

$180,000 01-2

A program of research to develop a new, unified computer based model for the behavior of materials which will be established upon explicit representations of the controlling internal processes and which will be completely quantitative. Emphasis directed to prediction of strength of ceramics containing surface damage due to machining and to prediction of the fracture behavior of transformation-toughened ceramics. Research will extend prior modeling advances in the areas of deformation and behavior of metals and alloys.

STANFORD UNIVERSITY (continued)

566. MECHANISMS OF HIGH TEMPERATURE CRACK GROWTH IN METALS AND ALLOYS

W. D. Nix
Dept. of Materials Science and Engineering
Phone: (415) 725-2605

$136,011 (18 months) 01-2

Study of the processes of creep crack extension in simple metals (Cu and Ni), examination of cavitation damage at crack tips using implanted intergranular cavities and intergranular segregation of Sb in Cu to permit grain boundary fracture in post-creep impact tests, study of the driving forces for crack growth and the temperature dependence of the growth process, examination of the effects of environments on creep crack growth in Ni alloys containing carbon, study of creep crack growth in 304 stainless steel containing different intergranular carbide distributions, theoretical studies of cavitation and crack growth.

[redacted] PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

R. Sinclair
Dept. of Materials Science and Engineering
Phone: (415) 723-1102

$ 29,728 (9 months) 01-3

Interactions occuring at the interface between CdTe with other materials, and the role of interfacial microstructure and microchemistry on the electrical properties of such CdTe containing heterojunctions. Effects of etching and heat treatment on surface, Schottky barriers, and heterojunctions formed on CdTe. Grain boundary characterization and passivation. Measurements include J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; and diffusion lengths. Scanning transmission electron microscopy and high resolution TEM analysis of heterojunction interfaces, lattice resolution and electron microdiffraction; XPS, Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition; magnetron sputtering; chemical vapor deposition; and closed-space vapor transport techniques.

STANFORD UNIVERSITY (continued)

568. FUNDAMENTAL STUDIES OF THE CHEMICAL VAPOR DEPOSITION OF DIAMOND

D. A. Stevenson
Dept. of Materials Science and Engineering
Phone: (415) 723-4251

$145,000 01-3

A study of the mechanism of growth of diamond coatings by enhanced chemical vapor deposition (ECVD). Primary emphasis on: a) influence of enhancement methods (hot filament with and without DC bias), b) rate of etching of graphite and diamond by atomic hydrogen, and c) relation between gas phase chemistry and diamond coating. Coating process characterization by optical and mass spectroscopy methods; coatings characterized by RHEED, Raman spectroscopy, SIMS, SEM, TEM, XRD, profilometry, hardness, laser scattering and hot-stage stress measurements.

569. A STUDY OF MECHANICAL PROCESSING DAMAGE IN BRITTLE MATERIALS

B. T. Khuri-Yakub
Dept. of Electrical Engineering
Phone: (415) 723-0718

$117,542 01-5

The proposed research will investigate machining damage in brittle materials, initially hot-pressed Si_3N_4, and the associated residual surface stresses. Nondestructive evaluation (NDE) techniques will be developed and applied to the measurement of the depth of shallow cracks, simulating machining damage, and local stress fields. An attempt will be made to correlate the damage with microstructural features and to determine a quantitative relation between damage and remaining strength.

STANFORD UNIVERSITY (continued)

570. A QUEST FOR A NEW SUPERCONDUCTING STATE

J. P. Coleman
Dept. of Chemistry
Phone: (415) 497-4648
W. A. Little
Dept. of Physics
Phone: (415) 497-4233

$110,000 03-1

Synthesis and characterization of organic conductors in which the conducting spine is encompassed by macrocyclic dyes. Experimental tests of excitonic superconductivity. Preparation of polymeric materials consisting of stacked or bridged-stacked metalloporphyrin or metallophthalocyanine complexes. Structural characterization using EXAFS and XANES at the Stanford Synchrotron Radiation Laboratory and X-ray powder and single crystal crystallography. Measurements of conductivity, photoconductivity, and magnetic susceptibility. Calculations using extended Huckel molecular and band theory.

STEVENS INSTITUTE OF TECHNOLOGY
Hoboken, NJ 07030

571. MOLECULAR INTERACTIONS AND MAGNETISM AT SOLID SURFACES

G. M. Rothberg
Dept. of Materials and Metallurgical Engineering
Phone: (201) 420-5269

$ 25,000 02-2

Continued development of the spin polarized extended X-ray absorption fine structure (SPEXAFS) measurements of magnetic properties of solids. Direct determination of the distance and temperature dependences of spin-spin correlations in bulk magnetic solids and on surfaces. Attempt to study electronic structure of magnetic superlattice films.

SYRACUSE UNIVERSITY
Syracuse, NY 13210

572. THE CATALYTIC REACTIVITY TO THIN FILM CRYSTAL SURFACES

R. W. Vook
Dept. of Physics
Phone: (315) 423-2564

$ 86,128 01-1

Investigate chemical reactions on heterogeneous thin-film surfaces consisting of a thick epitaxial film on which fractional to several average monolayers of another metal have been deposited. Use (111) Pd substrates with epitaxial (111) Cu as films and vice versa. Catalytic activity at high pressure as a function of overgrowth thickness. Desorption energies and desorption kinetics for the gaseous reactants, CO and O. Surface characterization by AES, LEED, and TEM/TED studies of film microstructure. Nature of the electronic structure of the thin film surfaces with and without gaseous adsorbates.

TEMPLE UNIVERSITY
Philadelphia, PA 19122

573. MIXED VALENT AND HEAVY-FERMIONS AND RELATED SYSTEMS

P. Schlottman
Dept. of Physics
Phone: (215) 787-7655

$172,000 (24 months) 02-3

Theoretical study of highly correlated Fermion systems. Bethe-Ansatz is used to solve the orbitally degenerate Anderson impurity model with finite Coulomb repulsion. The low temperature resistivity of a pair of impurities and the Kondo lattice, as well as the Kondo hole, is studied within a Fermi liquid approach. The generalization of Migdal-Kadanoff's renormalization group to heavy fermion systems is used to study the interplay of interactions leading to ordered phases in U and Ce compounds.

UNIVERSITY OF TENNESSEE
Knoxville, TN 37996-1600

574. STATISTICAL MECHANICS OF POLYMER SYSTEMS

J. Kovac
Dept. of Chemistry
Phone: (615) 974-3444

$ 94,690 03-1

Theoretical investigation of the equilibrium and dynamic behavior of high polymer systems over a broad range of concentration, temperature, and molecular weight. Particular areas of interest are the effect of excluded volume and entanglements on polymer dynamics and the origin of glass transitions. Methods of analysis include non-equilibrium thermodynamics, equilibrium and non-equilibrium statistical mechanics, and computer simulation.

575. INVESTIGATIONS OF THE EFFECTS OF ISOTOPIC SUBSTITUTION AND PRESSURE ON MISCRIBILITY IN POLYMER-POLYMER AND POLYMER-SOLVENT SYSTEMS

Alexander A. Van Hook
Dept. of Chemistry
Phone: (615) 974-5105

$117,904 03-2

Measurement of phase separation temperature and related properties as a function of isotopic labeling (H/D) and pressure in polymer-polymer and polymer-solvent systems. Comparison, through the use of statistical theory of isotope effects in condensed phases, of isotope effect and pressure effects on the thermodynamic properties of solution, including particularly the consolate properties. These measurements will be used to refine present molecular models of polymer-polymer and polymer-solvent interactions. The results will aid in the interpretation of neutron scattering data in H/D mixtures of polymers.

UNIVERSITY OF UTAH
Salt Lake City, UT 84112

576. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V SYSTEMS

G. B. Stringfellow
Dept. of Materials Science and Engineering
Phone: (801) 581-8387

$101,719 01-1

Detailed exploration of the phenomenon of ordering in III/V alloys with large positive enthalpies of mixing with emphasis on expanding the ordered structure domain size and increasing the degree of ordering. Electron microscopy characterization invoking lattice imaging and reflection electron microscopy. Microprobe analysis. Photoluminescence. Raman scattering. Hall effect. OMVPE. Candidate materials include $GaAs_{0.5}Sb_{0.5}$ and $Ga_{0.75}In_{0.25}As_{0.75}Sb_{0.25}$ (both grown on InP substrates), $Ga_{0.5}In_{0.5}As_{0.5}Sb_{0.5}$ (grown on InAs substrates), and superlattice structures between InAs and InP_xSb_{1-x} and between GaPSb and GaInPSb.

[redacted] FABRICATION, PHASE TRANSFORMATION STUDIES, AND CHARACTERIZATION OF $SIC-ALN-AL_2OC$

A. V. Virkar
Dept. of Materials Science and Engineering
Phone: (801) 581-5396

$115,156 01-1

Evaluation of phase equilibria and determination of phase transformation kinetics in the $SiC-AlN-Al_2OC$ system. Processing including hot pressing to achieve controlled precipitate morphology. X-ray diffraction and STEM analysis concerning phase equilibria, precipitate morphology, spinodal decomposition, grain boundaries, and the nucleation and growth of grain boundary phases. Establishment of relationship between composition/microstructure and creep behavior/fracture toughness.

578. ALUMINA REINFORCED TETRAGONAL ZIRCONIA (TZP) COMPOSITES

D. K. Shetty
Dept. Materials Science and Engineering
Phone: (801) 581-6449

$116,540 01-2

Study combined effects of transformation toughening and fiber reinforcement in the ceramic-composite $Al_2O_3-ZrO_2$. Fabricate, process, and characterize Al_2O_3 fiber reinforced tetragonal ZrO_2. Independent variables are temperature, pressure and fiber mixing. Elucidate composite microstructures, phase compositions and physicochemical properties. Use fiber coatings to alter interface bonding and electrical mechanical analog technique to track fracture problems unique to ceramic composite systems.

VIRGINIA COMMONWEALTH UNIVERSITY
Richmond, VA 23284

579. ELECTRONIC STRUCTURE AND GEOMETRIES OF SMALL COMPOUND METAL CLUSTERS

P. Jena
Dept. of Physics
Phone: (804) 367-1313
B. K. Rao
Dept. of Physics
Phone: (804) 367-1313
S. N. Khanna
Dept. of Physics
Phone: (804) 367-1313

$134,245 01-3

Theoretical studies of the structural and electronic properties of small atomic clusters of transition metal elements (Fe, Ni, V) interacting with H_2, O_2, CO, and NH_3 molecules as well as compound clusters involving alkali atoms, Al, Mg, and Cu. Studies of the equilibrium geometries, electronic charge and spin density distribution, local density of states, magnetic moment per atom, binding energies, and ionization potentials of "naked" homo-nuclear clusters using theoretical techniques (with atomic numbers of the instituent atoms as the only input) and following a total energy minimization procedure. Changes in these properties due to adsorption of H_2, O_2, CO, and NH_3. The results, with insights into the evolution of bulk and surface properties as clusters grow, compared with experimental data. Exploration of the influence of results on technological developments in the fields of catalysis, photochemical reactions, and production of new materials.

VIRGINIA STATE UNIVERSITY
Petersburg, VA 23803

580. CHARACTERIZATION OF SUPERCONDUCTING MATERIALS WITH MUON SPIN ROTATION

C. E. Stronach
Dept. of Physics
Phone: (804) 520-6153

$ 94,000 01-3

Use of muon spin rotation to characterize the magnetic states in high temperature and heavy-fermion superconductors. Investigate the relationship between magnetic ordering and superconductivity.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

581. STUDY OF THE EMBEDDED ATOM METHOD OF ATOMISTIC CALCULATIONS FOR METALS AND ALLOYS

R. A. Johnson
Dept. of Materials Science
Phone: (804) 924-6356

$ 83,000 01-1

Theoretical studies to (1) obtain a better physical insight into the relationship between the input data and the EAM model parameters, (2) study the effects variations of the EAM model parameters have on predicted material properties, and (3) use these results to assess the range of applicability of the EAM model and to improve its reliability within this range.

582. MICROSTRUCTURAL AND SEGREGATION EFFECTS ON THE TRANSFORMATIONS AND MECHANICAL PROPERTIES OF FE-C-X ALLOYS

G. L. Shiflet
Dept. of Materials Science
Phone: (804) 924-3226
T. H. Courtney
Dept. of Materials Science
Phone: (804) 924-6340

$ 53,232 01-2

This research addresses the cyclic fatigue behavior of low alloy multiphase steels. The aim is to establish the effect of microstructure on crack initiation and propagation in tensile and fatigue tests of steel with well-controlled and characterized microstructures. Parallel modelling of the phase stability and crack propagation.

583. SURFACE STRUCTURE AND ANALYSIS WITH SCANNING TUNNELING MICROSCOPY AND ELECTRON TUNNELING SPECTROSCOPY

R. V. Coleman
Dept. of Physics
Phone: (804) 924-3781

$120,000 02-2

Development of scanning tunneling microscopes operating at liquid nitrogen and liquid helium temperatures. Observation and surface analysis of charge density waves. Superconductivity and charge density wave coexistence. Inelastic electron tunneling spectroscopy and imaging of surface molecules. Thin oxide films and tunnel junction barriers. Development of a high magnetic field scanning tunneling microscope.

UNIVERSITY OF VIRGINIA (continued)

584. SUPERCONDUCTING MATERIALS

J. Ruvalds
Dept. of Physics
Phone: (804) 924-6796

$ 91,500 02-3

Theoretical investigation of the phenomena of superconductivity. High temperature superconductors with $T_c > 77$ Kelvin. Alloys, including the YBa-Cu-O series of materials. Reduced dimensionality study of electron-phonon coupling mechanisms. Electronic structure calculations, high magnetic critical field calculations. Possible metallic hydrogen theory with corrections for exchange and correlation contributions to physical properties. Development of models to guide the materials development.

WASHINGTON STATE UNIVERSITY
Pullman, WA 99164-2920

585. METAL INDUCED EMBRITTLEMENT

R. G. Hoagland
Dept. of Mechanical and Metallurgical Engineering
Phone: (505) 335-8280

$ 79,003 01-2

Study of metal-induced embrittlement. Crack growth measurements combined with microscopic examinations of fracture mechanics specimens to establish the relationship between crack extension and crystallographic orientation, to characterize competing crack tip reactions, and to assess plastic wake effects. Computer simulations of embrittlement mechanisms on an atomic scale. Aluminum, zinc, and cadmium embrittled by mercury, gallium, and indium.

WASHINGTON UNIVERSITY
St. Louis, MO 63130

586. NON-EMPIRICAL INTERATOMIC POTENTIALS FOR TRANSITION METALS, ALLOYS AND SEMICONDUCTORS

A. E. Carlsson
Dept. of Physics
Phone: (314) 889-5739

$ 82,000 02-3

Development of computational methods for calculation of interatomic potentials used in simplified tight-binding models of transition metals and their alloys. Extension beyond the tight-binding model. Interatomic potentials tested both by experimental data and density-of-states band calculations. Applied to surfaces and vacancies and subsequently used to calculate phase diagrams and the properties of dislocations and grain boundaries.

UNIVERSITY OF WASHINGTON
Seattle, WA 98195

587. CONTROLLED PRODUCTION AND CHARACTERIZATION OF METASTABLE INTERMETALLICS

M. J. Kaufman
Dept. of Materials Science and Eng.
Phone: (206) 543-7161

$ 95,000 01-1

Production and characterization of metastable intermetallic phases produced by non-equilibrium processing methods such as rapid solidification. Identification and development of processing strategies for controlled processing subsequent to metastable phase formation. Emphasis on rapidly solidified melt-spun ribbons and submicron powder particles; analysis carried out by electron microscopy, X-ray diffraction, differential scanning calorimetry, and differential thermal analysis. Alloy systems selected for study include Ge-Al, Ti-Al, Hf-Al, and Zr-Al.

UNIVERSITY OF WASHINGTON (continued)

588. X-RAY AND GAMMA-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls
Dept. of Physics
Phone: (206) 543-2778

$134,100 02-2

Investigate the structure of materials at high pressure using X-ray absorption near-edge spectroscopy (XANES), extended X-ray absorption fine structure (EXAFS), and gamma-ray (i.e. Mossbauer) spectroscopy. Emphasis is on the study of materials undergoing structural transformations with pressure such as the bcc-hcp martensitic transformation in metallic iron, and the bond angle changes in perovskites, particularly the high T_c superconducting oxides.

589. FUNDAMENTAL STUDIES OF ELASTOMERS

B. E. Eichinger
Dept. of Chemistry
Phone: (206) 543-1653

$115,000 03-1

Chemistry and physics of elasticity aimed towards an improved understanding of the properties of elastomers. The approach uses experimental, computational, and theoretical methods to investigate the relationship between network structure, viscoelastic behavior, and equilibrium properties. Networks that are cross-linked through coordination complexes are being produced, they will be used for a variety of studies, including small angle X-ray scattering and stress-strain measurements. Computer simulations of network formation are used to investigate the statistics that govern the microstructural features of elastomers. The theory of the shape distribution of polymer molecules is being developed in conjunction with a theory of the elastic free energy.

WEST VIRGINIA UNIVERSITY
Morgantown, WV 26506

590. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

B. R. Cooper
Dept. of Physics
Phone: (304) 293-3423

$ 75,401 03-1

Investigation of the crystallographic allotropes of elemental plutonium with detailed calculations of the electronic structure, including correlation effects and contributions to the lattice energy. Theoretical model based on hybridization of the 5f electrons with the band electrons. Studies of plutonium monopnictides and monochalcogenides, the plutonium alpha distorted fcc phase, magnetic ordering, electrical resistivity, and self-consistent surface electronic structure.

UNIVERSITY OF WISCONSIN/MADISON
Madison, WI 53706

591. STUDIES OF ALTERNATIVE-CRYSTALLIZATION-PHASE NUCLEATION

T. F. Kelly
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-1073

$ 75,000 01-1

This research will be directed toward understanding phase nucleation during rapid solidification of metallic alloys. Characterization of as-solidified structures conducted with electron and X-ray diffraction methods and coupled with analyses of solidification phenomena in order to elucidate thermodynamic and kinetic factors dominating homogeneous and heterogeneous phase nucleation. Initial studies will address binary Fe-base alloys.

UNIVERSITY OF WISCONSIN/MADISON (continued)

592. THE STABILITY OF AMORPHOUS METALS ON SEMICONDUCTOR SUBSTRATES

J. H. Perepezko
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-1578
J. D. Wiley
Dept. of Electrical and Computer Engineering
Phone: (608) 263-1643

$ 51,300 (7 months) 01-1

Stability of amorphous alloy films during diffusion and interdiffusion treatments. Atomic transport measurements by a combination of RBS and AES. Structural analysis by XRD and TEM. Electrical behavior of amorphous metal/semiconductor contacts including both interfacial electrical (Schottky barrier and ohmic) behavior and the stability of amorphous metallization against current induced degradation by electromigration. Examination of structural relaxation during post-deposition annealing.

593. THERMODYNAMICS AND KINETICS OF PHASE FORMATION OF THIN-FILM METAL ON GALLIUM ARSENIDE

Y. A. Chang
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 262-1821

$115,720 01-3

Investigate the thermodynamics and kinetics of phase formation for metal films deposited on GaAs. Investigation consists of (1) bulk phase equilibrium and thermodynamic determinations of selected Ga-As-M ternaries and the associated thermodynamics modelling and phase diagram calculations; (2) bulk diffusion-couple measurements of GaAs-M; and (3) lateral thin-film diffusion couple measurements of GaAs-M and thin-film studies of M on GaAs and of GaAs on M. Systems under investigation are Ga-As-Os, Ga-As-Pd, and Ga-As-W. Phase equilibrium determinations using X-ray diffraction, metallography, microprobe, differential thermal analysis (DTA) and differential scanning calorimetry (DSC). Thermodynamic properties for Ga-M compound phases measured using a solid-state emf method. Diffusion paths in GaAs-M determined by means of microprobe analysis with bulk diffusion couples. The thin-film lateral diffusion couples characterized primarily by electron microscopy. Reactions and phase formation in thin films of metal on GaAs and of GaAs on metal characterized by electron microscopy and a variety of thin-film compositional, microstructural, and crystallographic analysis.

UNIVERSITY OF WISCONSIN/MADISON (continued)

594. FUNDAMENTAL STUDIES OF NEW MAGNETIC HETEROSTRUCTURES: THEIR GROWTH, CRYSTALLOGRAPHIC STRUCTURE, MAGNETIC, AND ELECTRONIC PROPERTIES

M. Onellion
Dept. of Physics
Phone: (608) 262-3822

$110,000 02-2

Development of Magneto-Optic Kerr Effect (MOKE) instrument using time resolved synchrotron light for surface studies. Prepare thin Heusler alloy films, rare-earth films with epitaxial techniques. Characterize the films with angle-resolved photoemission and electron microscopy. Low and High Energy Electron Diffraction (HEED, LEED) techniques. Electron spin and energy analysis. Development of a scanning tunneling microscope.

595. MORPHOLOGICAL ANALYSIS OF IONOMERS

S. L. Cooper
Department of Chemical Engineering
Phone: (608) 262-1092

$105,200 03-2

Synthesis of ionomers with regular placement of ionic groups along the chain. Small angle X-ray scattering techniques used to probe shape, size, and arrangements of ionic aggregates in ionomers. Effect of casting solvent, compression molding and solution casting on morphology. Determination of aggregate dissociation temperature. Anomalous small angle X-ray scattering (ASAXS) to resolve source of zero-angle upturn in scattering intensity. Tensile properties to monitor the dramatic cation influence, the effect of water, trends within a chemical group and the effect of anion type. SANS experiments using deuterated polyols will measure temperature dependence, response to deformation and be interpreted for cation effects.

UNIVERSITY OF WISCONSIN/MILWAUKEE
Milwaukee, WI 53201

596. INELASTIC ELECTRON SCATTERING FROM SURFACES

S. Y. Tong
Dept. of Physics
Phone: (414) 963-5765

$ 99,248 02-3

Theory of the inelastic scattering of electrons, ions, and neutral atoms from elementary excitations at surfaces, and the development of theoretical descriptions of these excitations. Emphasis on electron energy loss from surface photons at both clean and adsorbate-covered surfaces. Studies of spin-flip scattering of low energy electrons from magnetic excitations at surfaces, and excitation of surface phonons by helium atoms. Strong emphasis on the quantitative comparison between the results of this program and experimental data. Tightly coupled effort between Professor Tong and Professor Mills at the University of California at Irvine.

YALE UNIVERSITY
New Haven, CT 06520

[redacted] MICROSTRUCTURAL DEPENDENCE OF THE CAVITATION DAMAGE FUNCTION IN F.C.C. MATERIALS

B. L. Adams
Dept. of Mechanical Engineering
Phone: (203) 432-4223

$ 85,932 01-2

Establish microstructural and stress state dependence of cavitation damage in F.C.C. metal alloys. Experimental and analytical studies to define a Cavitation-Damage Function under multi-axial loading. Technique involves measuring local crystallite orientations adjacent to grain boundaries of sectioned samples using Electron Backscattering Diffraction. Materials are type 304 stainless steel and copper alloys.

SECTION C

Small Business Innovation Research

PHASE I SBIR PROJECTS

The goal of the Phase I projects is to determine the technical feasibility of the ideas proposed.

CHRONOS RESEARCH LABORATORIES, INC.
4186 Sorrento Valley Blvd., Suite H
San Diego, CA 92121

600. RADIATION MODIFIED PYROELECTRIC CONVERSION MATERIALS

R. B. Olsen
Phone: (619) 455-8200

$ 49,990 (6 months) SBIR

The pyroelectric converter is a form of heat engine which directly transforms heat energy into electrical energy. The pyroelectric converter has the potential for low operating and maintenance requirements. High reliability and lifetime of this device are attainable because the pyroelectric converter does not require any solid moving parts.

The specific technical problem we will address is that of modifying the temperature range over which the pyroelectric converter materials can effectively operate.

Advanced pyroelectric conversion devices will operate at about 30 percent efficiency by incorporating the materials developed under Phases I and II of this proposal.

KMS Fusion, Inc.
P.O. Box 1567
Ann Arbor, MI 48106-1567

601. SYNTHESIS OF NEW METASTABLE ULTRAHARD MATERIALS

M. R. Wixom
Phone: (313) 769-8500

$ 49,992 (6 months) SBIR

The hardest materials available today are diamond and cubic boron nitride. Both of these materials exist as metastable phases which can be synthetically produced from much softer and cheaper starting materials such as graphite. One of the techniques for producing synthetic diamond or cubic boron nitride is shock-wave processing at pressures in the 10-200 GPa range. Theoretical arguments suggest that other as yet unsynthesized ultrahard materials may also be recoverable in metastable phases. The proposed research will use shock processing of several new starting materials in an attempt to recover new ultrahard compounds.

Materials & Electrochemical
Research (MER) Corporation
4233 South Fremont Avenue
Tucson, AZ 85714

602. HIGH TEMPERATURE ADVANCED STRUCTURAL CERAMICS

C. F. Chen
Phone: (602) 746-9442

$ 50,000 (6 months) SBIR

Current investigations have shown how reinforcement increased the fracture toughness of SiC-whisker/ceramic-matrix composites. However, it was found that the strength of the composites decreased as a result of flaws introduced with the whisker addition and the poor sinterability of Si_3N_4. External pressure has to be introduced (e.g., hot-press or hot-isostatic press) for eliminating the flaws. SiAlON ceramics can reach almost full density through pressureless sintering and it also offers the same significance in high temperature mechanical properties as that of Si_3N_4. Densification and strengthening by transient liquid phase sintering (TLPS) has been explored. However, combining whisker reinforcement with TLPS has not been demonstrated. This program utilizes unique sinterability of SiAlON, TLPS, and SiC Whisker reinforcement to obtain flaw free, homogeneous and high temperature (>1400^{o}C) strength composite through pressureless sintering.

OPTRA, Inc.
83 Pine Street
Peabody, MA 01923

603. LASER SURFACE PROFILOMETER FOR STEEP ASPHERIC SURFACES

M. Hercher
Phone: (617) 535-7670

$ 49,913 (6 months) SBIR

The development of an interferometric surface profilometer is proposed. Key Phase I performance specifications include precision and resolution for steep aspheric surfaces of $\pm$2.5nm in surface height measurement. A spatial resolution of $\pm$0.2mm, and the ability to handle surface slopes in the range $\pm 25^{o}$ with a linear trade-off between these two parameters. During Phase II it is anticipated that periscopic optics will be developed (to inspect the interior of cylindrical surfaces) and that improvements in spatial resolution may be achieved. The proposed instrument is based on the use of 2-frequency HeNe laser, and is an evolution from a breadboard instrument which has exhibited subnanometer height resolution and 2 micron spatial resolution.

ORDELA, Inc.
139 Valley Court
Oak Ridge, TN 37830

604. DEVELOPMENT OF A METHOD FOR GREATLY INCREASING THE COUNT-RATE CAPABILITY AND ENDURANCE OF POSITION-SENSITIVE DETECTOR SYSTEMS

M. K. Kopp
Phone: (615) 483-8675

$ 50,000 (6 months) SBIR

The principal objective of this research is the development of a novel method that will greatly increase the count-rate capability and endurance of position-sensitive detector systems without compromising spatial, angular, or energy resolution. Such a detector system is capable of removing some of the limitations imposed by present detectors on material research at synchrotron radiation facilities and intense neutron sources. The increase in count rate capability is possible by combining a detector technology that uses one output channel per pixel with a novel charge-centroid finding method that is capable of operating at count rates of 10^5 photons or neutrons per second per pixel. The detector endurance in high intensity source environments is improved because the low output charge requirement of 10^{-14}C per detected event increases detector life by mitigating erosion and radiation damage problems. Within the scope of Phase I, a prototypic, multiwire detector system will be instrumented to study this novel approach and determine its potential for advancing the state of the art of detectors for scattering and diffraction of neutrons and photons in materials science applications with high intensity sources. The results obtained will serve as a base for future development during Phase II of a new generation of position sensitive detectors for these applications.

THERMA-WAVE, Inc.
47734 Westinghouse Drive
Fremont, CA 94539

605. NONCONTACT HIGH-RESOLUTION THERMAL WAVE DETECTION OF SUPERCONDUCTIVE TRANSITIONS IN HIGH-T_c MATERIALS

A. Rosencwaig
Phone: (415) 490-3663

$ 50,000 (6 months) SBIR

Developments to date in the field of high-T_c superconductors have been very exciting. However, practical materials and devices are still far from a reality. The ceramic superconductors are heterogeneous multiphase materials, and their superconducting properties appear to be sensitively dependent on the local microscopic nature of the material. It would be of considerable value both to the theoretical understanding of this new phenomenon, and to the development of better superconductor materials if more were known about the relationship between the local superconducting properties and the local structural and chemical parameters. A novel method to detect the onset of superconductivity on a microscopic scale would employ a laser based thermal wave technique. Phase I will demonstrate the capability of this method to detect the onset on superconductivity in high-T_c superconductors in a noncontact, nondamaging fashion with micron-scale resolution. This will permit the Phase II development of a prototype thermal wave system to characterize the superconductive properties of high-T_c materials on a microscopic scale. The noncontact, nondamaging aspect of this characterization would allow subsequent examination of the same microscopic regions with other microprobe techniques to determine the relationship between local superconducting properties and local structural and chemical properties.

UNIVERSAL ENERGY SYSTEMS, Inc.
4401 Dayton-Xenia Road
Dayton, OH 45432

606. CLOSED-LOOP FIGURING OF MIRRORS

E. S. Buck
Phone: (513) 426-6900

$ 49,049 (6 months) SBIR

Universal Energy Systems, Inc. (UES) proposes to measure continuously the thickness of a mirror blank from the back side, thus permitting the continuous removal of material from the front side without the necessity of stopping work periodically to measure the material removed. The method of measurement employs an "acoustic micrometer" which uses extremely short pulses to achieve a precision of a small fraction of a micrometer. Temperature compensation will be addressed.

PHASE II SBIR PROJECTS

The Phase II projects are a continuation of the successful Phase I projects. The goal of the Phase II projects is to determine commercial feasibility.

CERAMATEC, INC.
2425 South 900 West
Salt Lake City, UT 84119

607. HIGH THERMAL CONDUCTIVITY SINTERED AlN

R. A. Cutler
Phone: (801) 972-2455

$416,635 (24 months) SBIR

Aluminum nitride (AlN) is an important candidate material for advanced packaging of integrated circuits. Phase I showed that it was possible to obtain high thermal conductivity in AlN ceramics by understanding the thermodynamic and kinetic factors governing the removal of oxygen from the AlN lattice. Thermal conductivities in excess of 200 W/mK were obtained with yttria as a sintering aid and conductivity in excess of 180 W/mK was achieved when dysprosia was added to AlN. The most significant achievement during Phase I was the identification of a low temperature processing approach that will allow AlN with high thermal conductivity to be processed at temperatures now used for alumina substrates. Phase II will further explore the thermodynamic and kinetic factors defined in Phase I, as well as demonstrate the low temperature sintering process. Rare earth oxide levels (or alkaline earth oxide levels) necessary for the attainment of thermal conductivities in excess of 200 W/mK will be identified. Free energies of formation for rare earth and alkaline earth oxide aluminates will be determined, where appropriate. The free energy of formation of the aluminates will be correlated with thermal conductivity measurements to show the effect of the thermodynamic driving force for oxygen removal. THe kinetics of oxygen removal will be further investigated by correlating grain size with thermal conductivity. Mathematical modeling of the moving grain boundary will allow unambiguous interpretation of kinetic data. The most important aspect of Phase II is the development of a proprietary process to allow for the rapid sintering of AlN ceramics with conventional sintering aids at temperatures similar to those presently used for the production of alumina substrates for the electronics industry.

CERAMATEC, INC. (continued)

608. NEW LOW THERMAL EXPANSION STRUCTURAL CERAMICS

S. Y. Limaye
Phone: (801) 972-2455

$498,858 (24 months) SBIR

During Phase I, a ceramic material composition was discovered that has a nearly flat thermal expansion curve from room temperature to 1200°C and an average thermal expansion of $-2.8 \times 10^{-7}/^{o}C$. The material was synthesized through substitutions into the $[NaZr_2(PO_4)_3]$ structure to engineer the thermal expansion characteristics. Parallel experiments on fabrication of related compositions resulted in a strength increase from 27 MPa for the baseline material to 110 MPa. A similar magnitude of increase was achieved in thermal shock resistance. The objectives of Phase II are to:
(1) continue composition modifications to achieve a material with a flat expansion curve with a bulk expansion between room temperature and 1200°C in the range -2×10^{-7} to $2 \times 10^{-7}/^{o}C$; (2) achieve a strength greater than 200 MPa; (3) increase the thermal shock resistance such that no strength degradation occurs for a T of 1200°C; (4) demonstrate reproducible powder synthesis and sample fabrication; and (5) evaluate the high temperature thermal and chemical stability of the improved ceramic materials.

SECTION D

Major User Facilities
(Large Capital Investment)

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, NY 11973

The National Synchrotron Light Source (NSLS) is the nation's largest facility dedicated solely to the production of synchrotron radiation. The facility has two electron storage rings: a vacuum ultraviolet (VUV) ring which operates at an electron energy of 750 MeV designed for optimum radiation at energies between 10 eV and 1 keV, and an X-ray ring which operates at 2.5 GeV to optimize radiation between 1 keV and 20 keV. Since each of the 30 X-ray and 17 VUV beam ports can be further split into two to four beam lines it will be possible, the NSLS facility has the capacity for running as many as 100 experiments simultaneously.

A total of six insertion devices will ultimately be installed on the X-ray and VUV rings. These devices, known as either wigglers or undulators, are special magnets which produce synchrotron radiation orders of magnitude brighter than is available from the conventional bending magnets and, in the case of wigglers, extend the range of useful photon flux to higher energies. The insertion devices are used for microscopy, holography, medical research, materials sciences, high energy and high Q resolution scattering, spectroscopy, and Transverse Optical Klystron (TOK) experiments.

The NSLS is a facility where a wide range of research techniques are being used by biologists, chemists, solid state physicists, metallurgists, and engineers for basic and applied studies. Among the techniques used are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, crystallography, photoemission, radiometry, lithography, microscopy, circular dichroism, photoabsorption, and infrared vibrational spectroscopy.

Proprietary research can be performed at the NSLS. The DOE has granted the NSLS a Class Waiver under whose terms the Proprietary User is obligated to pay the full cost recovery rate for NSLS usage. In return, the user has the option to take title to any inventions made during the proprietary research program and to treat as proprietary all technical data generated during the proprietary research program.

USER MODES

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in establishment of comprehensive long-range experimental programs. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines have been designed and instrumented by Participating Research Teams (PRTs). The PRTs are entitled to up to 75 percent of their beam line(s) operational time for a 3-year term.

Insertion Device Teams (IDTs) have been formed to design, fabricate, commission, and use wiggler and undulator beam lines. The conditions and terms are similar to those of the PRTs.

NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

General users are scientists interested in using existing NSLS facilities for experimental programs. They are scheduled by an independent beam time allocation committee for a percentage of operating time for each beam line. Liaison and utilization support is provided to the General User by the cognizant beam line.

A program is available to support faculty/student research groups performing experiments at the NSLS as General Users, or performing neutron experiments at the BNL High Flux Beam Reactor (HFBR). The program is designed to encourage new users of these facilities and defray expenses incurred during exploratory visits to BNL, and while conducting initial experiments at the NSLS and HFBR. It is aimed at university users having only limited grant support for their research.

PERSON TO CONTACT FOR INFORMATION

Susan White-DePace (516) 282-7114
User Administration Office (FTS) 666-7114
NSLS, Bldg. 725B
Brookhaven National Laboratory
Upton, NY 11973

NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

TECHNICAL DATA

STORAGE RINGS	KEY FEATURES	OPERATING CHARACTERISTICS
VUV	High brightness; continuous wavelength range (λ = 25 Å); 17 beam ports	0.75 GeV electron energy
X-ray	High brightness; continuous wavelength range (λ = 2.5 Å); 30 beam ports	2.5 GeV electron energy

RESEARCH AREA	WAVELENGTH RANGE (Å)	NUMBER OF INSTRUMENTS
Circular Dichroism	1400 - 6000	1
Energy Dispersive Diffraction	0.1 - 2.5	3
EXAFS, NEXAFS, SEXAFS	0.1 - 250	24
Gas Phase Spectroscopy/ Atomic Physics	0.6 - 14.6	3
Infrared Spectroscopy	$2.5 \times 10^4 - 1.2 \times 10^8$	2
Lithography/Microscopy/Tomography	0.6 - 15	6
Medical Research	0.37	1
Nuclear Physics	$2.5 \times 10^{-6} - 2.5 \times 10^{-4}$	1
Photoionization	0.6 - 12000	5
Radiometry		1
Reflectometry	20 - 55	1
Research & Development/ Diagnostics	white beam	11
Time Resolved Fluorescence	1000 - 12000	2
Topography	0.1 - 3	3
Transverse Optical Klystron	12.5 - 1250	1
VUV & X-ray Photoemission Spectroscopy	0.3 - 1280	27

NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

TECHNICAL DATA

RESEARCH AREA	WAVELENGTH RANGE (Å)	NUMBER OF INSTRUMENTS
X-ray Crystallography	0.3 - 6.2	9
X-ray Fluorescence	0.3 - 620	2
X-ray Scattering/ Diffraction	0.1 - 15.5	26

HIGH FLUX BEAM REACTOR

Brookhaven National Laboratory
Upton, New York 11973

The Brookhaven High Flux Beam Reactor (HFBR) operates at a power of 60 megawatts and provides an intense source of thermal neutrons (total thermal flux = 1.0 x 10^{15} neutrons/cm^2-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($\gamma > 4$ A). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure is also available. The emphasis of the research efforts at the HFBR has been on the study of fundamental problems in the fields of solid state and nuclear physics and in structural chemistry and biology.

USER MODE

Experiments are selected on the basis of scientific merit by a Program Advisory Committee (PAC), composed of the specialists in relevant disciplines from both within and outside BNL. Use of the facilities is divided between Participating Research Teams (PRT's) and general users. PRT's consist of scientists from BNL or other government laboratories, universities, and industrial labs who have a common interest in developing and using beam facilities at the HFBR. In return for their development and management of these facilities, each PRT is assigned up to 75 percent of the available beam time, with the remainder being reserved for general users. The PAC reviews the use of the facilities by the PRT's and general users and assigns priorities as required.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/ student research groups performing experiments at the National Synchrotron Light Source or at the HFBR. It is aimed at university users having limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

Rae Greenberg (516) 282-5564
Bldg. 510B FTS 666-5564
Brookhaven National Laboratory

HIGH FLUX BEAM REACTOR

TECHNICAL DATA

Instruments	Purpose and Description
5 Triple-axis Spectrometers (H4M, H4S, H7, H8, H9A)	Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 MeV, $< E_0 <$ 200 MeV Q range: $0.03 < Q < 10 Å^{-1}$
Small Angle Neutron Scattering (H9B)	Studies of large molecules. Located on cold source with 20 x 20 cm^2 position-sensitive area detector. Sample detector distance L < 2 meter. Incident wavelength 4 Å $< \lambda_0 <$ 10 Å
Diffractometer (H3A)	Protein crystallography 20 x 20 cm^2 area detector λ_0 = 1.57 Å
Small Angle Scattering (H3B)	Studies of small angle diffraction of membranes. Double multilayer monochromator 1.5 Å $< \lambda <$ 4.0 Å 2d detector with time slicing electronics and on-line data analysis.
2 Diffractometers (H6S, H6M)	Single-crystal elastic scattering 4-circle goniometer 1.69 Å $< \lambda_0 <$ 0.65 Å
1 Triple-axis Spectrometer (H5)	Inelastic scattering Diffuse scattering Powder diffractometry
2 Spectrometers (H1A, H1B)	Neutron capture studies Energy range: 0.025 eV $< E_0 <$ 25 KeV
<u>TRISTAN II (Isotope Separator)</u> (H2)	Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission
<u>Irradiation Facilities</u>	
7 Vertical Thimbles	Neutron activation; production of isotopes; thermal flux: 8.3 x 10^{14} neutrons/cm^2-sec; fast (> 1.0 MeV) flux: 3 x 10^{14} neutrons/cm^2-sec.

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Solid State and Chemistry Divisions
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, phase transitions, liquid structures, and crystal structures. The HFIR is an 85-MW, light-water moderated reactor. The central flux is 4 x 10^{15} neutrons/cm^2-sec, and the flux at the inner end of the beam tubes is slightly greater than 10^{15} n/cm^2-sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Three of these are unique within this country: the double-crystal small-angle diffractometer, the correlation chopper, and the wide-angle time-slicing diffractometer. Facilities are available for studies of materials at low and high temperatures, high pressures, and high magnetic fields.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an external review committee. It is expected that all accepted experiments will be scheduled within 6 months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be borne by the user. Financial assistance is available for the travel and living expenses of users from U.S. universities. Inexperienced users will normally collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full cost recovery, including a charge for beam time. A brochure describing the facilities and a booklet giving user procedures is available on request.

PERSON TO CONTACT FOR INFORMATION

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Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6031

(615) 574-5240
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NEUTRON SCATTERING AT THE HIGH FLUX ISTOTOPE REACTOR (continued)

Technical Data

Beam No.	Instrument and Operating Characteristics
HB-1	Triple-axis polarized-beam, Beam size - 2.5 by 3 cm max, Flux - 2.6 x 10^6 n/cm^2s at sample (polarized), Vertical magnetic fields to 5 T, Horizontal fields to 2 T, Variable incident energy (E_0)
HB-1A	Triple-axis, fixed E_0, E_0 = 14.7 MeV, Wavelength = 2.353 angstroms, Beam size - 5 by 3.7 cm max, Flux - 9 x 10^6 n/cm^2s at sample with 40 min collimation
HB-2A	Liquid diffractometer with linear position sensitive detector, Beam size - 1 by 3.4 cm max, Wavelength = 0.89 angstroms, Detector covers 130° scattering angle, Flux - 6.8 x 10^5 n/cm^2s at sample with 20 min collimation
HB-2, HB-3	Triple-axis, variable E_0, Beam size - 5 x 3.7 cm max, Flux - 10^7 n/cm^2s at sample with 40 min collimation
HB-3A	Double-crystal small-angle diffractometer, Beam size - 4 x 2 cm max, Wavelength = 2.6 angstroms, Flux - 10^4 n/cm^2s, Resolution - 4 x 10^{-5} angstroms^{-1}
HB-4A	Four-circle diffractometer, Beam size - 5 x 5 mm, Flux - 2 x 10^6 n/cm^2s with 9 min collimation, Wavelength = 1.1015 angstroms
	Wide-angle time-slicing diffractometer, Beam size - 2 x 3.7 cm max, Wavelength = 1.015 angstroms, Flux - 2 x 10^6 n/cm^2s with 9 min collimation, Curved linear position sensitive detector covering 130°
HB-4	Correlation chopper, Beam size - 5 x 3.7 cm, Flight path - 1.5 m, 70 detectors covering 130°, Variable E_0, Variable pulse width
	Powder Diffractometer (under construction), Beam size - 5 x 3.7 cm, 32 detectors with 6 min collimators

INTENSE PULSED NEUTRON SOURCE

Argonne National Laboratory
Argonne, Illinois 60439

IPNS is pulsed spallation source dedicated to research on condensed matter. The peak thermal flux after installation of the new target will be about 1.2×10^{15} n/cm^2 sec. The source has some unique characteristics that have opened up new scientific opportunities:

- o high fluxes of epithermal neutrons (0.1-10 eV)
- o pulsed nature, suitable for real-time studies and measurements under extreme environment

Two principal types of scientific activity are underway at IPNS: neutron diffraction, concerned with the structural arrangement of atoms (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties, and inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level. At the same time, it is expected that the facilities will be used for technological applications, such as stress distribution in materials and characterization of zeolites, ceramics, and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS, Building 360, Argonne National Laboratory. Neutron time for proprietary research can be purchased based on the full-cost recovery rate.

PERSONS TO CONTACT FOR INFORMATION

B. S. Brown, Division Director	(312) 972-4999
Argonne National Laboratory	FTS 972-4999
9700 South Cass Avenue	
Argonne, IL 60439	
T. G. Worlton, Scientific Secretary	(312) 972-8755
	FTS 972-8755

IPNS EXPERIMENTAL FACILITIES

Instrument (Instrument Scientist)	Range Wave-vector* (A^{-1})	Range Energy (eV)	Resolution Wave-vector (A^{-1})	Resolution Energy (eV)
Special Environment Powder Diffractometer (J. D. Jorgensen/K. Volin)	0.5-50	**	0.35%	**
General Purpose Powder Diffractometer (J. Faber/R. Hitterman)	0.5-100	**	0.25%	**
Single Crystal Diffractometer (A. J. Schultz)	2-20	**	2%	**
Low-Res. Medium-Energy Chopper Spectrometer (C.-K. Loong)	0.1-30	0-0.6	0.02 k_0	0.05 E_0
High-Res. Medium-Energy Chopper Spectrometer (D. L. Price)	0.3-9	0.1-4	0.01 k_0	0.02 E_0
Small Angle Diffractometer (J. E. Epperson/ P. Thiyagarajan)	0.006-0.35	**	0.004	**
Low-Temperature Chopper Spectrometer (P. E. Sokol--Penn State University, (814)863-0528, K. Herwig)	0.3-30	0.1-0.8	0.01 k_0	0.02 E_0
Polarized Neutron Reflectometer (G. P. Felcher)	0.0-0.07	**	0.0003	**
Quasi-Elastic Neutron Spectrometer (T. O. Brun)	0.42-2.59	0-0.1	~0.2	0.02 E_0

* Wave-vector, $k = 4\pi \sin\theta/\lambda$.
** No energy analysis.

INSTRUMENTS NOT YET IN THE USER PROGRAM

eV Spectrometer
Glass, Liquid and Amorphous Materials Diffractometer (under construction)
Neutron Reflectometer II (under construction)
Small Angle Diffractometer II (under development)

LOS ALAMOS NEUTRON SCATTERING CENTER

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The Los Alamos Neutron Scattering Center (LANSCE) facility is a pulsed spallation neutron source equipped with time-of-flight (TOF) spectrometers for condensed-matter research. Neutrons are produced by spallation when a pulsed 800-MeV proton beam, provided by the Los Alamos Meson Physics Facility (LAMPF) and an associated Proton Storage Ring (PSR), impinges on a tungsten target. To date, the PSR has achieved 65 percent of its design goal of 100-μA average proton current at 12-Hz repetition rate. When full current is achieved, LANSCE will have the world's highest, peak thermal flux for neutron scattering research.

Current research programs at LANSCE use the following instruments: a filter difference spectrometer (FDS) for vibrational spectroscopy by inelastic neutron scattering; a Laue-TOF single-crystal diffractometer (SCD); a high-intensity powder diffractometer (HIPD) for structural studies of liquids, amorphous materials, and crystalline powders; a neutron powder diffractometer (NPD) with the highest resolution in the U.S.; a constant-Q spectrometer (CQS) for the study of collective excitations, such as phonons and magnons; and a low-Q diffractometer (LQD) for small-angle scattering studies.

During the next 3 to 4 years, several new spectrometers will be installed at LANSCE, including: a chopper spectrometer for inelastic scattering measurements and Brillouin scattering; a neutron reflectometer with a polarized-neutron option; and a back-scattering spectrometer with a resolution of 10 μeV or better.

USER MODE

LANSCE provides neutron scattering facilities for several communities. At least 80 percent available beam time is used for condensed-matter research, while the remaining 20 percent is intended for internal use in support of the Laboratory's programmatic mission. Of the time available for condensed-matter work, most will be distributed to a formal user program, which will start in April 1988. Advice on experiments to be performed in this category will be provided by a Program Advisory Committee (PAC) held jointly with the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory. Scientists based at universities, national laboratories, and industry may apply for beam time by submitting short proposals for scrutiny by the PAC. No charge will be made for non-proprietary research.

CONTACT FOR USER INFORMATION

Dianne K. Hyer — (505) 667-6069 or
LANSCE Scientific Coordination and Liaison Office — (FTS) 843-6069
MS H805
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

LANSCE (continued)

TECHNICAL DATA (at design level)

Proton Source	LAMPF + PSR
Proton Source Current	1000 μA
Proton Source Energy	800 MeV
LANSCE Proton Current	100 μA
Proton Pulse Width	0.27 μs
Repetition Rate	12 Hz
Epithermal Neutron Current (n/eV.Sr.S)	$3.2 \times 10^{12}/E$
Peak Thermal Flux ($n/cm^2.S$)	1.7×10^{16}

INSTRUMENTS

32-m Neutron Powder Diffractometer (J. Goldstone, Responsible)	Powder Diffraction Wave vector 0.3-50 $Å^{-1}$ Resolution 0.13%
Single Crystal Diffractometer (P. Vergamini, Responsible)	Laue time-of-flight diffractometer Wave vectors 1-15 $Å^{-1}$ Resolution 2% typical
Filter Difference Spectrometer (J. Eckert, Responsible)	Inelastic neutron Scattering, vibrational spectroscopy Energy trans. 15-600 meV Resolution 5-7%
High Intensity Powder Diffractometer (A. Williams, Responsible)	Powder diffraction .7% resolution; liquids and amorphous materials diffraction 2% resolution
Constant-Q Spectrometer (R. Robinson, Responsible)	Elementary excitations in single crystal samples Energy resolution 1-3%
Low Q Diffractometer (P. A. Seeger, Responsible)	Small angle scattering at a liquid hydrogen cold source Wave vectors 0.003-1.0 $Å^{-1}$

STANFORD SYNCHROTRON RADIATION LABORATORY

Stanford University
Stanford, California 94309-0210

SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research in biology, chemistry, engineering, geology, materials science, medicine and physics. In addition to scientific research utilizing synchrotron radiation the Laboratory program includes the development of advanced sources of synchrotron radiation (e.g., insertion devices for the enhancement of synchrotron radiation as well as modifications of SPEAR and PEP). SSRL presently has 24 experimental stations. The radiation on 11 stations is enhanced by insertion devices providing the world's most intense X-ray sources.

Two of SSRL's experimental stations are located on the 16 GeV storage ring PEP. These lines provide the world's brightest continuous X-ray beams and, in addition to scientific research, will serve as development centers for future high-brightness beam line concepts.

The primary research activities at SSRL are:

X-ray absorption, small and large angle scattering as well as topographic studies of atomic arrangements in complex materials systems, including surfaces, extremely dilute constituents, amorphous materials and biological materials.

Soft X-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter.

Non-invasive angiography. X-ray lithography and microscopy. SSRL serves approximately 650 scientists from 114 institutions working on over 150 active proposals. A wide variety of experimental equipment is available for the user and there are no charges either for use of the beam or for the facility-owned support equipment. Proprietary research may be performed on a cost-recovery basis by special arrangement.

USER MODE

SSRL is a user-oriented facility which welcomes proposals for experiments from all qualified scientists. Over 75 percent of the beam time is available for the general user. Access is gained through proposal submittal and peer review. In the course of a year approximately 60 percent of all active proposals receive beam time. An annual Activity Report is available on request. It includes progress reports on about 100 experiments plus descriptions of recent facility developments. The booklet "SSRL User Guide" includes information on proposal submittal and experimental station characteristics.

STANFORD SYNCHROTRON RADIATION LABORATORY (continued)

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell (415) 926-3191
SSRL, Bin 69 PO Box 4349 (FTS) 462-3191
Stanford, CA 94309-0210

CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

SSRL presently has 22 experimental stations 21 of which are located on SPEAR and one on PEP. Nine of these stations are based on insertion devices while the remainder use bending magnet radiation.

	Horizontal Angular Acceptance (Mrad)	Mirror CutOff (KeV)	Monochromator	Energy Range (eV)	Resolution Δ/E	Approximate Spot Size HgtxWdth (mm)	Dedicated Instrumenation
INSERTION DEVICE STATIONS							
WIGGLER LINES - X-RAY							
End Stations							
IV-2 (8 pole)							
Focused	4.6	10.2	Double Crystal	2800-10200	-5x10^{-4}	2 x 6	
Unfocused	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	
VI-2 (54 pole)							
Focused	2.3	22	Double Crystal	2800-21000	-5x10^{-4}	2.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	
VII-2 (8 pole)							Six-circle Diffractometer
Focused	4.6	10.2	Double Crystal	2800-10200	-5x10^{-4}	2 x 6	
Side Stations							
IV-1	1.0	-	Double Crystal	2800-45000	-5x10^{-4}	2.0 x 20.0	
IV-3	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	Two-circle Diffractometer
VII-1	1.0	-	Curved Crystal	6000-13000	-8x10^{-4}	0.6 x 3.0	Rotation Camera
VII-3	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	
UNDULATOR LINES - VUV/SOFT X-RAY							
V-2	1.5	-	Rowland Circle-Multiple Grating	10-1200	≥7%	6.0 x 8.0	Angle Integrated e$^-$ Spectrometer
UNDULATOR LINES - X-RAY							
PEP 5B	Full	15.0	Double Crystal	12000-20000	-10^{-4}	0.6 x 6.0	
BENDING MAGNET LINES							
X-RAY							
I-4	2.0		Curved Crystal	6700-10800	0.3x10^{-3}	0.25 x 0.5	
I-5	1.0	-	Double Crystal	2800-30000	-10^{-4}	3 x 20	Area Detector/CAD-4
II-2 (focused)	4.8	8.9	Double Crystal	2800-8900	-5x10^{-4}	1 x 4	
II-3	1.0	-	Double Crystal	2800-30000	-5x10^{-4}	3 x 20	
II-4	1.0	-	None	3200-30000		3.5 x 18	
Lifetimes Port	1.8	-	None	1-6	Bandpass >10A	4.0 x .4	
VUV/SOFT X-RAY							
I-1	2.0		Grasshopper	32-1000	$\Delta\lambda$ = .1-.2A	1.0 x 1.0	
I-2	4.0		6m TGM	8-180	$\Delta\lambda$ = .06-3A	TBD	
III-1	2.0		Grasshopper	25-1200	$\Delta\lambda$ = .05-2A	1.0 x 1.0	
III-2	4.0		Seya-Namioka	5-50	$\Delta\lambda$ = .2-6A	TBD	
III-3	8-10	4.5	UHV Double Crystal (Jumbo)	800-4500	0.35-7 eV	2.0 x 4.0	
III-4	0.6		Multilayer	0-3000	White or $\Delta\lambda/\lambda$ = .3%	2 x 8	Vacuum Diffractometer/ Lithography Exposure Station
VIII-1	12		6m TGM	8-180	ΔK = .06-3A	TBD	Angle Resolved e$^-$ Spectrometer

SECTION E

Other User Facilities

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The National Center for Small-Angle Scattering Research (NCSASR) is supported by the National Science Foundation and the Department of Energy under an interagency agreement. The two main instruments available to users are the NSF-constructed 30-m small-angle neutron scattering facility (SANS) and the DOE-constructed 10-m small-angle X-ray scattering camera (SAXS). These instruments are intended to provide state-of-the-art capability for investigating structures of condensed matter on a global scale, e.g., from a few tens to several hundreds of angstroms. They are intended to serve the needs of scientists in the areas of biology, polymer science, chemistry, metallurgy and materials science, and solid state physics.

USER MODE

Beam time on these instruments is assigned, in general, on the basis of proposals submitted in advance. These are then reviewed by a panel of experts external to the Laboratory and are rated on the basis of scientific merit. When a favorable review has been received, a staff member of the NCSASR and the user agree, usually by telephone, on a time and duration for the experiment. Ordinary charges are borne by the Center, but extensive use of support facilities (shops, computing, etc.) must be paid by the user. Users may work in collaboration with one or more staff members if they wish, but such collaboration is not required. Proprietary experiments can be carried out after contractual agreement has been reached.

PERSONS TO CONTACT FOR INFORMATION

G. D. Wignall, SANS-NCSASR — (615) 574-5237
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NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Technical Data

30-m SANS Instrument Specifications

Monochromator: six pairs of pyrolytic graphite crystals
Incident wavelength: 4.75 angstroms or 2.38 angstroms
Wavelength resolution: $\Delta\lambda/\lambda = 6\%$
Source-to-sample distance: 8 m
Beam size at specimen: 0.5-3.0 cm diam
Sample-to-detector distance: 1.5-18.5 m
K range: $2 \times 10^{-3} < K = 4\pi\lambda^{-1} \sin\theta < 0.6$ angstroms^{-1}
Detector: 64 by 64 cm^2
Flux at specimen: 10^4-10^6 n/cm^{2}s depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite
Incident wavelengths: 1.542 angstroms (CuK α) or 0.707 angstroms (MoKα)
Source-to-sample distances: 0.5 - 5.0 m in 0.5 m intervals
Beam size at specimen: 0.1 cm by 0.1 cm (fixed)
Sample-to-detector distances: 1.0 - 5.0 m in 0.5 m intervals
K range covered: $3 \times 10^{-3} \leq K \leq 0.6$ angstroms^{-1} (CuK α)
$6 \times 10^{-3} \leq K \leq 1.2$ angstroms^{-1} (MoK α)
Flux at specimen: 10^6-10^7 photons per second on sample-irradiated area 0.1 by 0.1 cm, depending on source-sample-detector distances
Detector: 20- by 20-cm^2 (electronic resolution 0.1 by 0.1 cm^2)
Special features: deformation device for dynamic scattering experiments (time slicing in periods as short as 100 microseconds for oscillatory experiments or 10 seconds for transient relaxation experiments) and interactive graphics for data analysis

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory Electron Microscopy Center for Materials Research provides unique facilities which combine the techniques of high-voltage electron microscopy, ion-beam modification, and ion-beam analysis, along with analytical electron microscopy.

The cornerstone of the Center is a High Voltage Electron Microscope (an improved Kratos/AEI EM7) with a maximum voltage of 1.2 MV. This HVEM is interfaced to two accelerators, a National Electrostics 2 MV Tandem Ion Accelerator and a Texas Nuclear 100 kV ion accelerator, which can produce ion beams from 10 keV to 8 MeV of most stable elements in the periodic table. Procurement of a 650 kV injector is underway as a replacement for the Texas Nuclear accelerator. These instruments together comprise the unique High-Voltage Electron Microscope-Tandem Accelerator Facility. The available ion beams can be transported into the HVEM to permit direct observation of the effects of ions and electrons on materials. In addition to the ion-beam interface, the HVEM has a number of specialized features (see following page), which allow for a wide range of in situ experiments on materials under a variety of conditions.

In addition to the HVEM-Tandem Facility, the Center's facilities include a JEOL 100 CXII transmission and scanning transmission electron microscope (TEM/STEM), equipped with an X-ray energy dispersive spectrometer (XEDS), a Philips EM 420 TEM/STEM equipped with XEDS and an electron energy loss spectrometer (EELS) and a Philips CM30 with an XEDS. Procurement of an advanced Analytical Electron Microscope (AEM) is underway. This state-of-the-art, field emission gun ultra-high vacuum AEM will operate up to 300 keV and have the highest available microanalytical resolution with capabilities for XEDS, EELS, and Auger Electron Spectroscopy AES. As such, it will have substantially increased analytical capabilities for materials research over present-day instruments.

USER MODE

The HVEM-Tandem Facility is operated as a national resource for materials research. Qualified scientists wishing to conduct experiments using the HVEM/TANDEM facilities of the Center should submit a proposal to the person(s) named below. Experiments are approved by a Steering Committee following peer evaluation of the proposals. There are no use charges for basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH (continued)

PERSON(S) TO CONTACT FOR INFORMATION

E. A. Ryan (312) 972-5222
FTS 972-5222
and
N. J. Zaluzec (312) 972-5075
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Electron Microscopy Center for Materials Research
Materials Science and Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

TECHNICAL DATA

Electron Microscopes	Key Features
High-Voltage Electron Microscope Kratos/AEI EM7 (1.2 MeV)	Resolution 3.5 Å lattice Continuous voltage selection (100-1200 kv) Current density 15 A/cm^2 High-vacuum specimen chamber Negative-ion trap Electron and ion dosimetry systems Video recording system Ion-beam interface Specimen stages 10 - 1300 K Straining and environmental stages
Transmission Electron Microscope Philips EM 420 (120 keV)	Resolution 2.0 Å lattice Equipped with EELS, XEDS Specimen stages 30 - 400 K
Transmission Electron Microscope Philips CM 30 (300 keV)	Resolution 1.4 Å lattice Equipped with XEDS Specimen stages 30 - 400 K
Transmission Electron Microscope JEOL 100 CX (100 keV)	Resolution 3.4 Å lattice Equipped with STEM, XEDS Specimen stages 300 - 900 K
Analytical Electron Microscope Being procured (300 keV)	State-of-the-art resolution Ultra-high vacuum, Field Emission Gun Equipped with EELS, XEDS, AES, SIMS, LEED, etc.

Accelerators	
NEC Model 2 UDHS	Terminal voltage 2 MV Energy stability $\pm$250 eV Current density: H^+, 10 μA/cm^2 (typical) Ni^+, 3 μA/cm^2

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH (continued)

Electron Microscopes	Key Features
Texas Nuclear	Terminal voltage 100 kV Energy stability $\pm$300 eV Current density: He^+, 200 $\mu A/cm^2$ (typical) Ni^+, 2 $\mu A/cm^2$
NEC 650 kV Injector Being acquired	Terminal voltage 650 kV Energy stability $\pm$60 eV Current density: He^+, 100 $\mu A/cm^2$ (typical) Ar^+, 10 $\mu A/cm^2$

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

A wide range of facilities for use in materials science are available for collaborative research by members of universities or industry with ORNL staff members. The facilities include state-of-the-art electron microscopy, high voltage electron microscopy, atom probe/field ion microscopy, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include analytical electron microscopy [energy dispersive X-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS), and convergent beam electron diffraction (CBED)]. Surface analysis facilities include four Auger electron spectroscopy (AES) systems, and 0.4 and 5.0 Van de Graaff accelerators for Rutherford back-scattering and nuclear reaction techniques. Other equipment includes a mechanical properties microprobe (Nanoindenter), X-ray diffraction systems, rapid solidification apparatus, and various other facilities in the Metals and Ceramics Division.

USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, P. S. Sklad, I. Baker, C. B. Carter and K. Newport. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and current ORNL research. One ORNL staff member must be identified who is familiar with required techniques and will share responsibility for the project.

The SHaRE program provides technical help and limited travel expenses for academic participants through the Oak Ridge Associated Universities (ORAU).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik — (615) 574-5066, FTS 624-5066
Metals and Ceramics Division
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, Tennessee 37831

A. Wohlpart — (615) 576-3422, FTS 626-3422
Oak Ridge Associated Universities
P. O. Box 117
Oak Ridge, Tennessee 37831

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Facilities	Key Features	Operating Characteristics*
Hitachi HU-1000 HVEM, 0.3-1 MV	Cooling and heating stages, in situ deformation stages: video recording	Ten 4-h shifts/wk; In situ studies, electron irradiation studies
Philips EM400T/ FEG (AEM) 120 kV	EDS, EELS, CBED, STEM; minimum probe diam ~1 nm**	Ten 4-h shifts/wk; structural and elemental microanalysis
Philips CM12 AEM 120 kV	EDS, CBED, STEM; video recording**	Ten 4-h shifts/wk; structural and elemental microanalysis
JEOL 2000FX AEM 200 kV	EDS, CBED, EELS, STEM; examination of irradiated materials	Ten 4-hr shifts/wk; structural and elemental microanalysis
Philips CM30 AEM 300 kV	EDS, EELS, CBED, STEM; video recording**	Ten 4-h shifts/wk; structural and elemental microanalysis
JEM 120C TEM 120 kV	Polepiece for TEM of ferromagnetic materials	Ten 4-h shifts/wk; structural analysis
Atom Probe Field-Ion microscope	TOF atom probe, imaging atom probe, FIM, pulsed laser atom probe	Atomic resolution imaging: single atom analysis elemental mapping
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam; fracture stage; RGA; depth profiling elemental mapping	Surface analytical and segregation studies
Varian Scanning Auger Electron Spectroscopy System	5 micron beam; hot-cold fracture stage; RGA: depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Triple Ion-Beam Accelerator Facilities	400 kV, 2 MV, 4 MV Van de Graff accelerators sputter profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis

* Many instruments available off-hours (evenings, weekends) to qualified users.

** Stages for cooling, heating, and deformation available for Philips microscopes.

CENTER FOR MICROANALYSIS OF MATERIALS

Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

The Center operates a wide range of advanced surface chemistry, X-ray and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, microcrystallography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded from the MRL contracts of University of Illinois faculty, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research through a contract with a faculty member associated with the MRL, or by direct negotiation with the management of the Center. Direct user access to the equipment is also possible, for trained individuals. In all cases, the research carried out by users of the Center has to be in the furtherance of DOE objectives.

The equipment is made available on a flexible week-by-week booking scheme; if professional help is required, operating hours are 8-5, except by special arrangement. Fully qualified users can and do use the equipment at any time of day. Several of the instruments are maintained in almost continuous (24 hour) use.

The Center staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217) 333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

CENTER FOR MICROANALYSIS OF MATERIALS (continued)

In addition to the main items listed opposite, the Center also has other equipment: an electron microprobe, optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including seven ion-milling stations, a micro-ion mill, electropolishing units, sputter coaters, a spark cutter, ultrasonic cutter, diamond saw, dimpler, etc.

CENTER FOR MICROANALYSIS OF MATERIALS

Instruments	"Acronym"	Features and Characteristics
Imaging Secondary Ion Microprobe Cameca IMS 3f	SIMS	Dual ion sources (C_s^+, O_2^+). 1 μm resolution.
Secondary Neutral Mass Spectrometer Leybold Heraeus INA 3	SNMS	Quantitative analysis, Depth profiling.
Scanning Auger Microprobe Physical Electronics 595	Auger	Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector.
Scanning Auger Microprobe Physical Electronics 660	Auger	Resolution: SEM 25 nm Auger 60 nm
Scanning Auger Microprobe Physical Electronics 545	Auger	Resolution: SEM 3 μm.
X-ray Photoelectron Spectrometer Physical Electronics 5400	XPS	Resolution: 50 meV, 180^o spherical analyzer, Mg/Al and Mg/Ag anodes
X-ray Photoelectron Spectrometer Physical Electronics 548	XPS	Double pass CMA. ESCA and Auger Specimen temp. to 1550K
Transmission Electron Microscope Philips EM430 (300kV)	TEM	EDS, EELS, STEM
Transmission Electron Microscope Philips EM420 (120kV) Stage (30K).	TEM	EDS (windowless), EELS, STEM, Cathodoluminescence, Cold
Transmission Electron Microscope Philips EM400T (120kV)	TEM	EDS. Heating, cooling stages.
Transmission Electron Microscope JEOL 4000EX (400 kV)	TEM	For environmental cell use. Straining stages
Scanning Transmission E.M. Vacuum Generators HB5 (100kV)	STEM	0.5 nm probe, field emission gun, EDS, EELS.
Scanning Electronic Microscope Hitachi S800	SEM	Field Emission Gun Resolution 2nm, EDX
Scanning Electron Microscope JEOL JSM 35C (35kV)	SEM	5 nm resolution, EDX, channeling and backscattering patterns.

CENTER FOR MICROANALYSIS OF MATERIALS (continued)

Instruments	"Acronym"	Features and Characteristics
Rutherford Backscattering (in-house construction) (3 MeV)	RBS	Two work stations, channeling
X-ray Equipment	X-ray	
Elliott 14 kW high brilliance source		4-circle diffractometer.
Rigaku 12 kW source		Small angle camera. EXAFS.
Several conventional sources		Lang topography, Powder cameras, etc.

Rigaku D/Max-11B Computer Controlled Powder Diffractometer

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

This program utilizes a new approach for fundamental materials research. The combined techniques of ion implantation doping, ion-induced mixing, and pulsed-laser processing are utilized to alter the near-surface properties of a wide range of solids in ultrahigh vacuum. In situ analyses by ion beam, surface, and bulk properties techniques are used to determine the fundamental materials interactions leading to these property changes. Since both ion implantation doping and pulsed-laser annealing are nonequilibrium processes, they can be used to produce new and often unique materials properties not possible with equilibrium processing. These nonequilibrium techniques are also equally useful to modify surface properties for practical applications in areas such as friction, wear, corrosion, catalysis, surface hardness, solar cells, semiconducting devices, superconductors, etc.

This program has emphasis on long-range basic research. Consequently, most collaborative research involving scientists from industries, universities, and other laboratories has been the investigation of new materials properties possible with these processing techniques or the determination of the mechanisms responsible for observed property changes. In most instances such research projects identify definite practical applications and accelerate the transfer of these materials alteration techniques to processing applications.

COLLABORATIVE RESEARCH

User interactions are through mutually agreeable collaborative research projects between users and research scientists at ORNL which utilize the unique alteration/analysis capabilities of the SMAC facility. It should be emphasized that the goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application and not to provide routine service alterations or analyses.

PERSON TO CONTACT FOR INFORMATION

S. P. Withrow
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6048

(615) 576-6719
FTS 626-6719

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

Technical Data

Accelerators	Operating Characteristics
2.5-MV positive ion Van de Graaff	0.1-2.5 MeV; H, ^4He, ^3He, and selected gases. Beam current ~10-500 microamps
1.7-MV tandem	0.8-3.4 MeV H; 0.8-5.1 MeV ^3He, ^4He; negative ion sputtering source for heavy ion beams of selected species up to 10 MeV
10-200-KV high-current ion implantation accelerator	Most ion species; 1 milliamp singly charged, microamps doubly and triply charged 1-100
80-500-kV high-current ion implantation accelerator	Installation in late 1988
Lasers	
Pulsed Excimer Laser (0.249 micrometer)	20×10^{-9} s; 1.0 joule/pulse
Facilities	
UHV analysis chambers	Several chambers; vacuums 10^{-6}-10^{-11} torr; multiple access ports; UHV goniometers (4-1300K)
In situ analysis capabilities	Ion scattering, ion channeling, ion-induced nuclear reactions and characteristic X-rays; LEED, Auger, ion-induced Auger;
Combined ion-beam and laser processing	Laser and ion beams integrated into same UHV chambers
Scanning electron microscope	JEOL-840 with energy dispersive X-ray analysis

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94551-0969

Optical techniques, primarily Raman spectroscopy and nonlinear optical spectroscopy, are being developed and used to study the behavior of materials exposed to high-temperature environments. Emphasis is on the in situ use of these techniques to identify chemical species present on surfaces during attack and the resultant effects on structural phases of the material under study. Both pulsed and continuous-wave lasers at various wavelengths throughout the visible and ultraviolet regions are available for excitation of Raman scattering, which can be analyzed with 1 and 2 dimensional photon counting detectors, multichannel diode array detectors, and gated detection. Ultrahigh vacuum chambers, laboratory furnaces, and combustion flow reactors are available that are equipped with convenient optical access, providing realistic environments for in situ measurements. Real-time measurements are complemented by post-exposure techniques such as Raman spectroscopy with sputtering and low-energy electron diffraction.

Nonlinear optical spectroscopies, in particular second harmonic generation, have been developed for the detection of monolayer and submonolayer coverages of surfaces. Picosecond Nd:YAG and dye lasers (10 pps) and a high repetition rate (1kHz) Nd:YAG laser provide pulsed excitation at a variety of wavelengths. Extension of capabilities to the sub-hundred-femtosecond range is underway. Analysis of samples in UHV-based systems provides careful control over the high temperature modification of surfaces.

USER MODE

Interactions include: (1) collaborative research projects with outside users, and (2) technology transfer of new diagostic approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the persons listed below. If further investigations appear reasonable, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government laboratories have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSONS TO CONTACT FOR INFORMATION

Marshall Lapp, High Temp. Interfaces Div. (8342) — (415) 294-2435, FTS 234-2435

Gary B. Drummond, Ass't to the Director (8301) — (415) 294-2697, FTS 234-2697
Sandia National Laboratories
Livermore, California 94551-0969

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Technical Data

Instruments	Key Features	Comments
Raman Surface Analysis System	UHV Chamber; Raman system with Ar laser; triple spectrograph, diode array detector and 2-D imaging photon counting detector; Auger; sputtering capability	Simultaneous Raman and sputtering. Raman system capable of detecting 2 nm thick oxides. Sample heating up to 1100 C.
Raman Microprobe	Hot stage; Raman system with Ar, Kr lasers; scanning triple spectrometer.	1-2 micron spatial resolution. Hot stage can handle corrosive gases.
Raman High-Temperature Corrosion System	Furnace; Raman system with Ar, Kr, Cu-vapor lasers Nd:YAG; triple spectrograph and diode array detector.	Pulsed lasers gated detection for blackbody background rejection. Furnace allows exposure to oxidizing, reducing, and sulfidizing environments.
Combustion Flow Reactors	Raman system with Ar, Kr, Cu-vapor. lasers; triple spectrograph and diode array detector.	Vapor and particulate injection into flames. Real-time measurements of deposit formation.
Electrochemical Surface Modification System	Electrochemical cell; Raman system. with Ar, Kr, Cu-vapor lasers; triple spectrograph and diode array detector.	Electrochemical cell with recirculating pump and nitrogen purge.
Nonlinear Optical Spectroscopy of Surfaces System	Picosecond Nd:YAG and dye lasers, 10 pps; UHV chamber equipped with LEED, Auger, sputtering, and quad. mass spectroscopy.	Monolayer and submonolayer detection of high temperature hydrogen and oxygen adsorption and nitrogen segregation on alloys.
Nonlinear Optical Spectroscopy of Electrochemical Systems	Nd:YAG laser, 1kHz rep rate; electrochemical cell.	Monolayer and submonolayer detection of metals, oxygen, and hydrogen adsorption at electrodes.

MATERIALS PREPARATION CENTER

Ames Laboratory
Iowa State University
Ames, Iowa 50011

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section, the Materials Referral System and Hotline (MRSH), and the High-T_c Superconductivity Information Exchange. The Analytical Section has extensive expertise and capabilities for the characterization of materials, including complete facilities for chemical and spectrographic analyses, and selected services of this section are available to the research community. The purpose of MRSH is to accumulate information from all known National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community. The High-T_c Superconductivity Information Exchange provides a centralized site for rapid dissemination of up-to-date information on high-temperature superconductivity research. It publishes the newsletter, High-T_c Update, twice-monthly without charge, as both hard copy and electronic mail.

MATERIALS PREPARATION CENTER (continued)

USER MODE

Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Frederick A. Schmidt, Director, Materials Preparation Center.

Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquiries should be directed to Tom Wessels, MRSH Manager, (515) 294-8900.

High-T_C Superconductivity Information Exchange

The newsletter, High-T_C Update, is published twice-monthly and available without charge as either hard copy or electronic mail. Inquiries should be directed to Ellen O. Feinberg, (515) 294-3877.

TECHNICAL DATA

Materials

Scandium	Titanium	Magnesium	Thorium
Yttrium	Vanadium	Calcium	Uranium
Lanthanum	Chromium	Strontium	
Cerium	Manganese	Barium	
Praseodymium	Zirconium		
Neodymium	Niobium		
Samarium	Molybdenum		
Europium	Hafnium		
Gadolinium	Tantalum		
Terbium	Tungsten		
Dysprosium	Rhenium		
Holmium			
Erbium			
Thulium			
Ytterbium			
Lutetium			

MATERIALS PREPARATION CENTER (continued)

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt, Director (515) 294-5236
Materials Preparation Center
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

NATIONAL CENTER FOR ELECTRON MICROSCOPY

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

The National Center for Electron Microscopy (NCEM) was formally established in the fall of 1981 as a component of the Materials and Molecular Research Division, Lawrence Berkeley Laboratory.

The NCEM provides unique facilities and advanced research programs in the United States for electron microscopy characterization of materials. Its mission is to carry out fundamental research and maintain state-of-the-art facilities and expertise. Present instrumentation at the Center includes a conventional 650-kV Hitachi electron microscope installed in 1969 in the Hearst Mining Building on the University of California Berkeley campus, a 1.6-MeV Kratos microscope dedicated largely for in situ work, a 1-MeV JOEL atomic resolution microscope at 1.5 angstrom point-to-point (ARM), a high-resolution feeder microscope (JEOL 200 CX), and a 200-kV analytical microscope (JEOL 200 CX) equipped with a thin window, high-angle X-ray detector, and an energy loss spectrometer. Facilities for image simulation, analysis and interpretation are also available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. J. J. Hren, Chairman; J. M. Gibson, D. A. Howitt, F. Ponce, J. Barry, C. W. Allen, and L. E. Thomas; internal members are G. Thomas, T. L. Hayes, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be a sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer, and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore
National Center for Electron Microscopy
Mail Stop: 72-150
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

(FTS) 451-5006, or
(415) 486-5006

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characterization
KRATOS 1.5-MeV Electron Microscope	Resolution 3 Å (pt-pt) environmental cell; hot, cold, straining stages, CBED, video camera.	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. LaB_6 filament. Max. beam current 70 amp/cm^2. 3-mm diameter specimens.
JEOL 1-MeV Atomic Resolution Microscope	Resolution < 1.5 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, ±40° biaxial tilt with height control.	50-80 hrs/week, 400 kV-1 MeV, LaB_6 filament, 3-mm diameter specimens.
Hitachi 650-kV Electron Microscope	General purpose resolution 20 Å environmental cell, straining stage.	Installed in 1969. Max. voltage 650 kV conventional HVEM, 3-mm diameter specimens.
JEOL 200 CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only.	200 kV only, LaB_6 filament, 2.3-mm or 3-mm diameter specimens.
JEOL 200 CX dedicated Analytical Electron Microscope	Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, EELS spectrometer.	100 kV-200 kV LaB_6 filament, state-of-the-art resolution; 3-mm diameter specimens.

LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The Low-Temperature Neutron Irradiation Facility (LTNIF) is a user-oriented facility for the study of radiation effects in materials. It is available for qualified experiments at no cost to users. The LTNIF provides a combination of high radiation intensities and special environmental and testing conditions that have not been previously available in the U.S. A closed-cycle liquid-helium refrigerator and other cooling equipment allows samples to be held at temperatures between 3.2 and 800 K during irradiations and tests. The irradiation chamber fits into a vacant fuel element position in the reactor core to optimize fast neutron flux. Spectrum modifiers will be designed and constructed as needed to optimize gamma-ray or thermal-neutron flux. In many cases, experimental characterizations can be carried out in the irradiation cryostat. Alternatively, cold transfer to auxiliary equipment is available. The conditions available in the LTNIF are useful in a wide variety of radiation effects studies, ranging from measurements of defect production and characterization in materials to the production of nonequilibrium phases of solids and the evaluation of structural materials for use in fusion reactors.

USER MODE

The LTNIF is operated as a user-oriented facility. In addition, a limited number of collaborative research projects will be undertaken by the staff. Time on the facility is assigned on the basis of proposals submitted in advance. Staff members are aided in the selection of user experiments by an advisory/program committee. Because of the special safety requirements of operating in a reactor, acceptance of proposals requires an evaluation by appropriate ORNL safety personnel in addition to the usual evaluation for scientific merit. Use of the reactor and cryostat is at no cost to users, but extensive use of shops and other support facilities must be paid by the user.

PERSONS TO CONTACT FOR INFORMATION

H. R. Kerchner — (615) 574-6270, FTS 624-6270
Solid State Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37831-6030

NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Technical Data

Refrigeration:	Minimum temperature, 3.2 K (low reactor power) Capacity at 5 K, 70 W (removes nuclear heat generated in cryostat and a 100 g experiment at full reactor power)
Radiation (preliminary):	Fast neutrons, (E > 0.1 MeV), 2×10^{17} n/m^2s Thermal neutrons, 1.5×10^{17} n/m^2s Gamma rays, 0.3 w/g (in Al)
Dimensions:	Irradiation chamber, 38 mm diam x 250 mm long Test chamber, 198 mm diam x 300 mm long

SECTION F

Summary of Funding Levels

SUMMARY OF FUNDING LEVELS

During the fiscal year ending September 30, 1988, the Materials Sciences total support level amounted to about $___ million in operating funds (budget outlays) and $____ million in equipment funds. The following analysis of costs is concerned only with operating funds (including SBIR) i.e., equipment funds which are expended primarily at Laboratories are not shown in the analysis. Equipment support for the Contract and Grant Research projects is included as part of the operating budget.

1. <u>By Region of the Country</u>

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Northeast............... (CT, DC, DE, MA, MD, ME, NJ, NH, NY, PA, RI, VT)	38.9	27.1
(b) South................... (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	11.4	17.6
(c) Midwest................. (IA, IL, IN, MI, MN, MO, OH, WI)	20.3	29.2
(d) West.................... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	29.4	26.1
	100.0	100.0

2. By Discipline:

	Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-)	58.5	33.4
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	30.4	31.2
(c) Materials Chemistry (Budget Activity Numbers 03-)	11.1	10.4
(d) Facility Operations	---	25.0
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including laboratories where graduate students are involved in research to a large extent, i.e., LBL, Ames and IL)...	34.0
(b) DOE Laboratory Programs...........	64.7
(c) Industry and Other................	1.3
	100.0

4. By Laboratory and Contract and Grant Research:

	Total Program (%)
Ames Laboratory	5.3
Argonne National Laboratory	15.7
Brookhaven National Laboratory	20.5
Idaho National Engineering Laboratory	0.1
Illinois, University of (Materials Research Laboratory)	2.8
Lawrence Berkeley Laboratory	9.3
Lawrence Livermore National Laboratory	1.4
Los Alamos National Laboratory	5.2
Oak Ridge National Laboratory	15.5
Pacific Northwest Laboratory	1.1
Sandia National Laboratory	3.9
Solar Energy Research Institute	0.1
Stanford Synchrotron Radiation Laboratory	1.1
Contract and Grant Research	18.0
	100.0

SECTION G

Index of Investigators, Materials, Techniques, Phenomena, and Environment

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

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INVESTIGATORS

MATERIALS, TECHNIQUES, PHENOMENA, AND ENVIRONMENT

The numbers in parenthesis at the end of each listing of Abstract numbers gives for each topic the percentage of prorated projects, the percentage of funding, and the percentage of individual projects respectively. The prorated projects and the funding levels are based on estimates of the fractions of a given project devoted to the topic. The operating funds for fiscal year 1986 were $172,491,000. The number of projects is 453.

MATERIALS

Actinides-Metals, Alloys and Compounds
005, 013, 047, 049, 051, 076, 161, 200, 205, 242, 255, 355, 374, 413
522, 523, 547, 573, 590
(1.37, 0.88, 4.19)

Aluminum and its Alloys
006, 017, 078, 100, 107, 110, 115, 116, 118, 130, 147, 201, 223, 234
291, 352, 368, 371, 384, 403, 416, 420, 423, 430, 473, 502, 542, 585
587, 607
(1.74, 0.89, 6.62)

Alkali and Alkaline Earth Metals and Alloys
081, 163, 242, 404, 443, 451, 493
(0.35, 0.20, 1.55)

Amorphous State: Liquids
055, 134, 139, 247, 298, 418, 421, 437, 438, 484, 487, 503, 526, 545
575
(1.32, 0.97, 3.31)

Amorphous State: Metallic Glasses
001, 040, 044, 075, 078, 106, 107, 131, 145, 157, 190, 191, 201, 223
228, 234, 255, 276, 298, 363, 371, 432, 478, 506, 532, 558, 592
(1.77, 1.95, 5.96)

Amorphous State: Non-Metallic Glasses (other than Silicates)
046, 051, 114, 125, 126, 153, 232, 276, 298, 350, 367, 393, 401, 435
438, 478, 483, 486, 491, 499, 500, 515, 550, 574
(1.48, 1.42, 5.30)

Amorphous State: Non-Metallic Glasses (Silicates)
011, 051, 123, 200, 262, 275, 298, 350, 368, 372, 435, 438, 491, 515
532, 555, 561
(1.37, 1.67, 3.75)

<u>Nitrides</u>
011, 019, 020, 053, 126, 163, 167, 170, 204, 231, 244, 264, 350, 456
478, 485, 486, 560, 569, 577, 601, 607
(1.08, 0.90, 4.86)

<u>Oxides: Binary</u>
019, 041, 042, 046, 050, 052, 055, 074, 074, 079, 081, 114, 124, 125
127, 149, 152, 164, 167, 168, 170, 204, 223, 225, 231, 247, 292, 350
351, 360, 367, 389, 393, 402, 403, 406, 411, 419, 425, 441, 444, 445
446, 451, 455, 456, 465, 466, 473, 474, 478, 479, 486, 502, 508, 509
510, 514, 528, 529, 533, 535, 548, 551, 563, 565, 567, 571, 578
(4.79, 2.98,15.23)

<u>Oxides: Non-Binary, Crystalline</u>
019, 041, 045, 047, 050, 073, 079, 123, 124, 133, 149, 152, 155, 167
168, 200, 206, 220, 223, 231, 243, 244, 247, 292, 350, 366, 393, 398
402, 403, 404, 409, 412, 419, 424, 431, 441, 446, 447, 452, 453, 454
456, 465, 466, 479, 483, 501, 508, 514, 521, 528, 546, 565, 580, 607
608
(3.91, 2.83,12.58)

<u>Polymers</u>
020, 083, 140, 169, 204, 208, 209, 229, 234, 237, 245, 255, 260, 265
354, 358, 380, 381, 382, 414, 425, 428, 434, 439, 468, 480, 482, 491
497, 505, 515, 517, 518, 540, 570, 574, 575, 589, 595, 600
(4.94, 2.90, 8.83)

<u>Platinum Metal Alloys (Platinum, Palladium, Rhodium, Irridium, Osmium, Ruthenium)</u>
014, 042, 109, 135, 147, 163, 170, 291, 395, 407, 422, 475, 572, 593
(1.04, 0.66, 3.09)

<u>Quantum Fluids and Solids</u>
012, 046, 051, 076, 134, 157, 159, 160, 207, 228, 364, 373, 417, 418
436, 460, 475
(1.21, 1.07, 3.75)

<u>Radioactive Waste Storage Materials (Hosts, Canister, Barriers)</u>
123, 355, 454, 456, 483, 537
(0.46, 0.10, 1.32)

<u>Rare Earth Metals and Compounds</u>
001, 002, 003, 005, 007, 008, 010, 013, 014, 016, 047, 051, 075, 076
146, 157, 161, 163, 205, 206, 228, 230, 242, 374, 401, 442, 475, 481
490, 522, 546, 549, 573, 584, 594
(2.16, 1.96, 7.73)

TECHNIQUES

<u>Work Functions</u>
507
(0.04, 0.00, 0.22)

<u>X-Ray Scattering and Diffraction (wide angle crystallography)</u>
008, 015, 019, 021, 041, 042, 048, 049, 050, 053, 054, 077, 079, 083
123, 134, 136, 153, 166, 168, 169, 190, 200, 201, 204, 221, 236, 245
255, 290, 353, 365, 375, 376, 377, 384, 386, 405, 411, 414, 415, 419
429, 438, 442, 443, 444, 451, 454, 459, 462, 469, 473, 479, 481, 490
491, 493, 495, 507, 514, 533, 538, 556, 560, 570, 577, 592, 593
(4.02, 2.69,15.23)

<u>X-Ray Scattering (small angle)</u>
048, 123, 153, 173, 234, 255, 298, 363, 437, 439, 468, 491, 497, 499
512, 577, 589
(1.32, 1.19, 3.75)

<u>X-Ray Scattering (other than crystallography)</u>
015, 046, 049, 060, 077, 173, 221, 245, 255, 298, 426, 430, 444, 451
477, 490, 496, 518, 551, 553
(1.13, 1.72, 4.42)

<u>X-Ray Photoelectron Spectroscopy</u>
019, 021, 022, 041, 057, 060, 070, 081, 083, 118, 142, 168, 170, 173
202, 238, 262, 298, 392, 424, 425, 464, 486, 491, 508, 561, 567
(1.30, 1.89, 5.96)

PHENOMENA

Electronic Structure - Metals including amorphous forms
013, 016, 019, 021, 047, 049, 051, 078, 081, 132, 135, 163, 201, 205
206, 220, 235, 298, 363, 395, 413, 442, 481, 495, 506, 519, 523, 530
547, 584, 594
(1.72, 2.16, 6.84)

Electronic Structure - Non-metals including amorphous forms
041, 050, 078, 111, 114, 126, 132, 139, 160, 206, 296, 380, 396, 401
427, 435, 465, 476, 478, 485, 488, 489, 501, 505, 508, 514, 525, 530
543, 570, 586
(2.08, 0.82, 6.84)

Erosion
502
(0.07, 0.03, 0.22)

Grain Boundaries
002, 004, 008, 042, 053, 070, 072, 074, 074, 100, 115, 118, 125, 167
168, 201, 220, 222, 223, 224, 236, 256, 261, 290, 291, 350, 352, 359
365, 377, 402, 406, 408, 409, 410, 415, 416, 424, 429, 442, 446, 449
450, 452, 463, 467, 470, 481, 492, 493, 501, 516, 520, 521, 535, 542
544, 551, 563, 567, 577, 597
(3.53, 2.38,13.69)

Hydrogen Attack
113, 115, 116, 118, 119, 122, 204, 276, 357, 467, 521
(0.60, 0.30, 2.43)

Ion Beam Mixing
040, 043, 044, 106, 168, 191, 223, 227, 239, 240, 244, 367
(0.71, 1.77, 2.65)

Laser Radiation Heating (annealing, solidification, surface treatement)
058, 105, 111, 146, 191, 192, 204, 232, 236, 239, 240, 276, 432, 559
(0.86, 1.53, 3.09)

Magnetism
002, 003, 005, 008, 010, 012, 014, 016, 047, 049, 051, 075, 077, 081
126, 153, 157, 161, 206, 220, 228, 230, 235, 372, 374, 380, 383, 413
414, 427, 442, 453, 460, 461, 475, 481, 488, 519, 522, 523, 524, 546
547, 557, 571, 573, 580, 594
(3.36, 2.56,10.60)

Martensitic Transformations and Transformation Toughening
010, 015, 041, 075, 120, 167, 190, 399, 404, 447, 503, 511
(0.60, 0.56, 2.65)

ENVIRONMENT

MAJOR FACILITIES: OPERATIONS

Pulsed Neutron Sources (Operations)
059, 203, 210
(0.66, 5.17, 0.66)

Steady State Neutron Sources (Operations)
084, 248
(0.44, 7.83, 0.44)

Synchrotron Radiation Sources (Operations)
049, 085, 204
(0.66, 8.02, 0.66)