DOE/ER-0447P
Dist. Category UC-404

March 1990

Materials Sciences Programs

Fiscal Year 1989

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, and Advanced Energy Projects 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, Polymers 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 1989 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

PUBLICATIONS

DOE Materials Sciences Programs 1988, September 1988 (DOE/ER-0348)[a]

A partial discussion of some (but not all inclusive) research needs and opportunities is available as follows:

Clusters and Cluster-Assembled Materials (1989)[d]
Mechanisms and Physics of Crack Growth: Application to Life Prediction (1986)[a]
Basic Research in Ceramic and Semiconductor Science at Selected Japanese Laboratories (1989)[a]
Molecular Monolayers and Films (1986)[b]
Micromechanisms of Fracture (1987)[a]
Bonding and Adhesion at Interfaces (1985)[c]
Novel Methods for Materials Synthesis (1984)[c]
Theory and Computer Simulation of Materials Structures and Imperfections (1984)[a]
Materials Preparation and Characterization Capabilities (1983)[a]
Critical and Strategic Materials (1983)[a]
Coatings and Surface Modifications (1983)[c]
High Pressure Science and Technology (1982)[a]
Scientific Needs of the Technology of Nuclear Waste Containment (1982)[a]
Radiation Effects (1981)[a]
Condensed Matter Theory and the Role of Computation (1981)[a]
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

Scientific User Facilities, a National Resource[a] (In press)
Centers for Collaborative Research[a]
Materials Sciences Division - Long Range Plan (1984)[a]
Special Instrumentation Research Opportunities for Fundamental Ceramic Science at DOE[e]

---

a Available in limited quantities from the Division of Materials Sciences by calling (301) 353-3426, -3427, or -3428.
[b] Published in Langmuir
[c] Published in Materials Science and Engineering
[d] Published in Journal of Materials Research
[e] Published in Ceramic Bulletin, 67, 8, August 1988

OFFICE OF BASIC ENERGY SCIENCES
Division of Materials Sciences

Division of Materials Sciences

Director: I. L. Thomas

Taree Foltz - Secretary
(301) 353-3427

Metallurgy and Ceramics Branch

Chief: R. J. Gottschall

Joanne Csordas - Secretary
(301) 353-3428

J. B. Darby, Jr.
A. L. Dragoo.
J.L. Routbort 1/
R. W. Heckel 2/
W. J. Weber 3/
D. W. Keefer 4/

Solid State Physics and Materials Chemistry Branch

Chief: B. C. Frazer

Christie Goodrich - Secretary
(301) 353-3426

R. D. Kelley
J. J. Smith
M. Leiser
C. R. Klee
C. C. Herrick 5/

Notes:

1/ On detail from Argonne National Laboratory
2/ On assignment from Michigan Technological University
3/ On detail from Pacific Northwest Laboratory
4/ On detail from Idaho National Engineering Laboratory
5/ 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 grants (mostly with Universities), 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 distributions of funding, and Section G has various indexes.

The FY 1989 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 1989 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. Foltz, J. Csordas, and C. Goodrich.

TABLE OF CONTENTS

SECTION A - LABORATORIES

SECTION B - Grant Research

SECTION C - Small Business Innovation Research

SECTION D - Major User Facilities

TABLE OF CONTENTS (Con't)

Page

SECTION E - Other User Facilities

SECTION F - Funding Levels

SECTION G - Index

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
R. B. Thompson - (515) 294-7864/9649

Metallurgy and Ceramics - 01

O. Buck - (515) 294-4446

1. Analysis of Interfaces
A. J. Bevolo
(515) 294-5414 **01-1**
$149,000

Studies of interface structure and composition using Auger, EELS, 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 grain boundary segregation in irradiated steels, cast irons, V-Ti based alloys, and high T_c superconductors. Local chemical state information from Auger lineshape analysis. Electronic structure of heavy fermion metals and binary transition metal alloys. Surface segregation in Ni and Pd based binary transition metal solid-solution alloys.

2. Solidification Microstructures
R. K. Trivedi, L. S. Chumbley,
R. W. McCallum, J. D. Verhoeven
(515) 294-5869 **01-1**
$400,000

Studies of solidification processes and their applications to technologically important materials. Theoretical modeling of microstructural evolution and correlation between microstructures and processing conditions. Rapid solidification processing by the laser treatment of materials and by highly undercooled fine droplets. Development of microstructure/processing maps. Study of interface kinetics and the effect of crystaline anisotropy on the microstructure evolution. Directional solidification in organic materials such as succinonitrile, pivalic acid, carbontetrabromide, hexachleotyhane, t-butanol and napthalene. Directional solidification studies on segregation 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.

3. Analysis of Microstructures
J. D. Verhoeven, A. J. Bevolo,
L. S. Chumbley, R. W. McCallum
(515) 294-9471 **01-1**
$596,000

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.

4. Martensitic Phase Transformations
C. T. Chan, B. N. Harmon,
K. M. Ho, C. Stassis
(515) 294-5082 **01-2**
$428,000

First principles calculations of electronic structure and total energies to study the order parameters, transformation paths, activation energies, and basic physics leading to analysis and control of the transformation. Detailed study of anharmonic couplings and their manifestation in phonon spectra preceding the transformation. Application of molecular dynamics using realistic interatomic potentials. Study of prototypical systems: Na, NiTi, NiAl, Ba, Zr, etc.

5. Mechanical Metallurgy
W. A. Spitzig, B. Biner, J. Kameda
(515) 294-5082 **01-2**
$475,000

Studies of the effects of environment and stress on the mechanical properties of metals. Effects of hydrogen on cracking in alloys under uniaxial and cyclic loading conditions. Interstitial effects on strength and ductility in both nonhydrogenated and hydrogenated V, Nb, and Ta. High-temperature-induced intergranular cracking in Ni base alloys. Effects of radiation-induced defects and solute segregation on intergranular 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.

6. Rare Earth and Related Materials
K. A. Gschneidner, Jr.
(515) 294-7931 **01-3**
$355,000

Study the behavior of rare earth materials in the extreme regime of low temperatures (down to 0.5 K) and high magnetic fields (up to 10T). This includes heat capacity, magnetic properties, electrical resistivity measurements. Examine the systematics of phase formation, or the variation of physical properties to understand various physical phenomena, such as bonding, alloy theory, structure of materials.

7. Nde Measurement Techniques
O. Buck, B. Biner, R. B. Thompson
(515) 294-4446 **01-5**
$347,000

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 crack tip shielding and its influence on crack growth rate and detectability. Acoustic microscopy techniques for high resolution studies of microstructure and defects. Effects of fatigue damage, stress and microstructure on magnetic properties, particularly Block wall motion.

8. Fundamentals Of Processing Of Bulk High Tc Superconductors
R. W. McCallum, J. D. Verhoeven
(515) 294-4736 **01-5**
$684,000

Investigation of the role of microstructure in the bulk superconducting properties of high T_c oxides. Control of microstructure using information obtained from phase diagram studies. Phase diagram dependence on rare earth and oxygen partial pressure. Interaction of materials with CO_2. Study of fine grained dense polycrystalline materials. Effects of processing induced defects on the bulk superconducting properties.

9. Advanced Materials and Processes
F. A. Schmidt, I. E. Anderson
(515) 294-5236 **01-5**
$633,000

Development of advanced processes for preparing special metals. Development of new melting procedures for preparing Cu-Nb, Cu-Ta, Cu-Mo, and Cu-Ta-W alloys. New thermite reduction process for preparing rare earth-iron alloys and for producing permanent magnet and magnetostrictive alloys. 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.

10. Scientific and Technological Information Exchange
F. A. Schmidt, E. O. Feinberg, T. E. Wessels
(515) 294-5236 **01-5**
$207,000

Dissemination of information to the scientific and industrial communities. Publication of High-Tc 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 - (515) 294-7712

11. Neutron Scattering
W. A. Kamitakahara, C. Stassis, J. Zarestky
(515) 294-4224 **02-1**
$428,000

Magnetic properties of high temperature superconductors (La_2CuO_4 ...). Study of the lattice dynamics, thermodynamic properties, and structural transformations of metals at high temperatures, 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}). Lattice dynamics of amorphous semiconductors.

12. New Materials and Phases
F. Borsa, D. C. Johnston, C. A. Swenson, D. R. Torgeson
(515) 294-5435 02-2
$590,000

Synthesis and characterization of new high T_c superconductors and related oxides. Study of the physical properties of these new materials, such as phase equilibria and high temperature behavior. Properties of new phases including magnetic susceptibility, transport properties, heat capacity, crystallographic phase transformations, coexistence of superconductivity and magnetic order. Modeling and analysis of the data using appropriate theories. 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 high T_c superconductors, phase transitions, and hydrogen embrittlement of refractory metals and alloys.

13. Superconductivity
D. K. Finnemore, J. E. Ostenson
(515) 294-3455 02-2
$450,000

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, 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.

14. X-ray Diffraction Physics
A. Goldman
(515) 294-3585 02-2
$227,000

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.

15. Optical, Spectroscopic, and Surface Properties Of Solids
D. W. Lynch, C. G. Olson, M. Tringides
(515) 294-3476 02-2
$470,000

Electron photoemission, inverse 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, copper-oxide-based superconductors, O on W. Fundamental studies of surface roughening and annealing, island growth, etc. using LEED line shape analysis.

16. Semiconductor Physics
H. R. Shanks, J. Shinar
(515) 294-8706 02-2
$230,000

Preparation and characterization of thin films, rf sputter desposition of amorphous semiconductors including αSi, αSi-C, αGe, αGe-C and crystalline AlN. Also diamond-like thin films. 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 of semiconductors and polymers using DLTS, SCLC, ODMR, and C-V on Schottky barriers.

17. Superconductivity Theory
J. R. Clem
(515) 294-4223 02-3
$169,000

Electrodynamic behavior of the high-temperature copper-oxide superconductors, especially while carrying electrical currents in magnetic fields. Anisotropy of critical fields, internal magnetic field distributions, and magnetization. Granularity effects using Josephson-coupled-grain models. Flux pinning, critical currents, thermally activated flux flow, noise, ac and high-frequency losses. Surface, interface, grain-boundary, and proximity effects.

18. Optical and Surface Physics Theory
R. Fuchs, K.-M. Ho
(515) 294-1960 **02-3**
$130,000

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).

19. Electronic And Magnetic Properties
B. N. Harmon, C. T. Chan, K.-M. Ho, M. Luban, C. Soukoulis
(515) 294-7712 **02-3**
$470,000

Magnetic properties of new high T_c superconductors. Theoretical studies of bulk and lattice dynamical properties of materials using first principles total energy calculations. Anharmonic interaction, lattice instabilities, phase transformation, electron-phonon interaction, and superconductivity. Equations of state (pressure and temperature). Hydrogen-metal interactions. Electron localization in quasi-periodic and 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. Localization of light in dielectrics. Theoretical modeling of quantum dot nanostructures.

Materials Chemistry - 03
P. A. Thiel - (515) 294-2770

20. Synthesis and Characterization Of New Materials
J. D. Corbett, R. A. Jacobson, R. E. McCarley
(515) 294-3086 **03-1**
$445,000

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.

21. Ceramics and Polymers
T. J. Barton, M. Akinc, K. Woo
(515) 294-7655 **03-2**
$462,000

Synthesis of silicon-nitrogen polymers. Study of controlled thermal decomposition of preceramic polymers. Development of thermal and photo-chemical 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. Polymers with metal-metal bonding.

22. **High Temperature Chemistry of Refractory Materials**
H. F. Franzen, J. W. Anderegg
(515) 294-5773 03-3
$242,000

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.

23. **Surface Chemistry**
P. A. Thiel, K. G. Baikerikar, R. S. Hansen, D. C. Johnson
(515) 294-2770 03-3
$510,000

Study of lubrication phenomena. Decomposition pathways and products of fluorinated ethers at surfaces. Mechanisms of corrosive oxidation of metals. Mechanisms of oxidative corrosion 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. 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. Techniques used include low energy electron diffraction, Auger electron spectroscopy, electron energy loss spectroscopy, temperature programmed desorption, electron-stimulated desorption, ring-disk and modulated hydrodynamic voltammetry.

Argonne National Laboratory

9700 South Cass Avenue
Argonne, IL 60439
Physical Research: F. Y. Fradin - (708) 972-3504/(FTS) 972-3504
Advanced Photon Source: D. M. Moncton - (708) 972-7950/(FTS) 972-7950

Metallurgy and Ceramics - 01

B. Dunlap - (708) 972-4925/(FTS) 972-4925

24. **Electron Microscopy Center For Materials Research**
N. J. Zaluzec, C. W. Allen
(708) 972-5075/(FTS) 972-5075 01-1
$1,522,000

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 hydrogenation effects. HVEM specimen stages are available for heating (1300 K), cooling (10 K), straining, resistivity and gaseous environments. Ion-beam interface with 650 kV ion accelerator and 2 MV tandem accelerator available for in situ implantations and irradiations. Approximately 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 microanalytical resolution and sensitivity. Fundamental studies of electron-solid interactions and microcharacterization of materials, using TEM, STEM, XEDS, and EELS are conducted at present on conventional transmission electron microscopes (JEOL 100CX, Philips EM420, and Philips CM30).

25. Basic Ceramics
D. J. Lam, S.-K. Chan, M. V. Nevitt, S. J. Rothman, J. L. Routbort, B. W. Veal
(708) 972-4966/(FTS) 972-4966 **01-3**
$1,305,000

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) spectroscopic 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.

26. Interfacial Studies
K. L. Merkle, J. N. Mundy
(708) 972-4990/(FTS) 972-4990 **01-3**
$716,000

Experimental 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. Grain boundary diffusion 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.

27. Irradiation and Kinetic Effects
L. E. Rehn, R. C. Birtcher, M. A. Kirk, N. Q. Lam, P. R. Okamoto, H. Wiedersich
(708) 972-5021/(FTS) 972-5021 **01-4**
$1,199,000

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. Ion channeling in High T_c materials. Radiation-induced segregation to internal and external defect sinks. Radiation-enhanced diffusion. Effects of irradiation on alloy composition, microstructure, grain growth, superconductivity, and amorphization. Displacement cascades. Inert-gases in solids. Effects of amorphization 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 changes. Ion-beam analysis. Radiation sources include HVEM-2MV Tandem facility and 650kV ion accelerator.

28. High Tc Superconductor Development
G. W. Crabtree, K. Goretta, R. B. Poeppel, J. L. Routbort, D. Shi
(708) 972-5509/(FTS) 972-5509 **01-5**
$478,000

Development of a short length, current-carrying, ceramic superconductor made by tape-casting, extrusion, powder-in-tubes, thick-film techniques, co-evaporation, 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 field. Collaborative research with scientists at Ames Laboratory and Brookhaven National Laboratory.

29. Amorphous and Nanophase Materials
L. E. Rehn, J. Eastman, P. R. Okamoto, R. W. Siegel
(708) 972-5021/(FTS) 972-5021 **01-5**
$689,000

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, by displacement damage of intermetallic compounds by electron and ion beams, and by hydrogenation. Elastic property measurements in ordered, disordered and amorphous alloys. In situ high-voltage electron microscopy studies of the morphology and kinetics of 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.

Solid State Physics - 02

B. Dunlap - (708) 972-4925/(FTS) 972-4925

30. Neutron and X-ray Scattering
J. D. Jorgensen, J. E. Epperson, G. P. Felcher, R. Kleb, D. L. Price, S. Susman
(708) 972-5513/(FTS) 972-5513 **02-1**
$1,645,000

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, liquid alloys and molten salts, surface magnetism, alloy decomposition, polymer interfaces, coarsening processes, distributions with deep inelastic scattering, and fast ion transport in solids.

31. Two-Dimensional Materials
S. D. Bader, M. B. Brodsky, M. Grimsditch, E. Moog
(708) 972-4960/(FTS) 972-4960 **02-2**
$869,000

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.

32. Superconductivity and Magnetism
G. W. Crabtree, B. D. Dunlap, A. J. Fedro, K. E. Gray, D. G. Hinks, L. C. Smedskjaer
(708) 972-5538/(FTS) 972-5538 **02-2**
$1,378,000

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.

33. Ceramic Epitaxy and Multilayer Structures
D. J. Lam, H. L. Chang
(708) 972-4966/(FTS) 972-4966 **02-2**
$445,000

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 experimental 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.

34. Photon Science at Synchrotrons
G. K. Shenoy, E. E. Alp, J. C. Campuzano, M. Ramanathan, H. You
(708) 972-5537/(FTS) 972-5537 **02-2**
$455,000

Experimental investigations using various synchrotron radiation sources of electronic and structural properties of materials. X-Ray edge systematics to understand the chemical structure of materials. Fermi surface, X-ray absorption and structural studies of high temperature superconductors. Measurements of the structure of surfaces and interfaces using surface scattering techniques. Study of electrochemical interfaces.

35. Condensed Matter Theory
D. D. Koelling, R. Benedek, R. K. Kalia, M. Norman, K. J. Strandburg, P. Vashishta
(708) 972-5507/(FTS) 972-5507 **02-3**
$1,103,000

Condensed matter theory in statistical physics, electronic band theory and many body effects. Quantum Molecular Dynamics modeling of low electrondensity materials. Classical Molecular Dynamics modeling of chalcogenide glasses. Transport and structural transformations in ionic conductors. Electronic structure calculations of narrow band metal and alloy systems. Phenomenological incorporation of fluctuation phenomenon effects on electronic structure, resulting in huge mass enhancements and superconductivity in heavy fermion materials. Positron annihilation effects in metals and alloys. Non-linear optimization techniques for electronic structure. Studies of the new high T_c superconductors. Models for quasicrystal structure.

36. Modeling and Theory of Interfaces
D. Wolf, S. Phillpot, S. Yip
(708) 972-5205/(FTS) 972-5205 **02-3**
$267,000

Computer simulation of the physical properties of solid interfaces, such as grain and interphase boundaries, thin films and superlattices, involving both atomistic simulation methods (lattice statics and dynamics, molecular dynamics, Monte-Carlo). The atomistic simulations are used to determine, for example, the structure, free energy and elastic properties 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.

37. Ultra-High Field Superconductors
K. E. Gray, R. T. Kampwirth
(708) 972-5525/(FTS) 972-5525 **02-5**
$371,000

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, and new low-temperature in situ techniques are being investigated. 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 and superconducting properties. Layered NbN/AlN films exhibiting 4-5 times higher critical current density than NbN at high fields will also be addressed.

Materials Chemistry - 03
B. Dunlap - (708) 972-4925/(FTS) 972-4925

38. Chemical and Electronic Structure
J. M. Williams, M. A. Beno, K. D. Carlson, G. M. Frankenbach, U. Geiser, A. M. Kini, A. J. Schultz, H. H. Wang
(708) 972-3464/(FTS) 972-3464 **03-1**
$1,186,000

New materials synthesis and characterization focusing on synthetic organic metals and superconductors based on BEDT-TTF (bis-ethylenedithiotetrathio-fulvalene) and various new organic electron 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) single crystal X-ray diffraction instrument.

39. Thermodynamics of Ordered and Metastable Materials
M. Blander, L. A. Curtiss, M. L. Saboungi
(708) 972-4548/(FTS) 972-4548 **03-2**
$509,000

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.

40. Interfacial Materials Chemistry
V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, A. R. Krauss
(708) 972-4547/(FTS) 972-4547 03-2
$496,000

Basic research on interfacial phenomena in two forefront scientific fields of materials science: (1) molecular sieve materials and their application in heterogeneous catalysis and (2) novel techniques for the preparation and characterization of high-critical-temperature (T_c) superconductors in thin-film form. Investigations of the synthesis and basic properties of the newer families of metal- and silicon-substituted aluminophosphate molecular sieves, including novel materials that present abundant opportunities for new catalyst design and development and for exploitation of other useful properties. Exploratory research that employs a panoply of sophisticated techniques, including neutron scattering, nuclear magnetic resonance, electron spin resonance, infrared spectroscopy, and molecular dynamics calculations. Production and characterization of multicomponent thin films and layered structures by computer-controlled sequential deposition with in situ annealing and oxidation processes as part of an integrated fabrication cycle. Use of atomic oxygen and oxygen ion beam modification to produce high temperature superconductor (HTSC) films with little or no high temperature annealing. Atomic layer-by-layer fabrication of Bi and Tl-based HTSCs. Production of superlattice structures for electronic applications and thin-film optoelectronic devices. Production of layered silicide structures for electrical contacts in high density electronic devices. Basic surface studies of as-grown superconducting thin films; basic studies of growth processes for multicomponent thin films.

41. Aqueous Corrosion
V. A. Maroni, L. A. Curtiss, N. C. Hung, C. A. Melendres, Z. Nagy, M. J. Pellin, R. M. Yonco
(708) 972-4547/(FTS) 972-4547 03-2
$639,000

Basic research aimed at elucidating fundamental aspects of aqueous corrosion under conditions of temperature and pressure (300°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, Raman-gain, second harmonic generation and X-ray 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.

42. Particle and Photon Interactions with Surfaces
D. M. Gruen, W. F. Calaway, A. R. Krauss, G. J. Lamich, M. J. Pellin, C. E. Young
(312) 972-3513/(FTS) 972-3513 03-3
$1,016,000

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.

43. Molecular Identification for Surface Analysis
D. M. Gruen, K. R. Lykke, M. J. Pellin
(708) 972-3513/(FTS) 972-3513 03-3
$250,000

Surface analysis of the molecular composition of complex solids using Fourier transform ion cyclotron resonance spectroscopy coupled with resonant and "soft" laser ionization methods. The solid surfaces to be investigated include conducting polymers, plastics, and other high molecular weight materials. One aspect of the study involves the diffusion and fate of additives such as plasticizers and UV stabilizers in polymers.

Facility Operations - 04

44. Intense Pulsed Neutron Source Program
B. S. Brown, J. M. Carpenter, R. K. Crawford, A. Rauchas, J. Richardson, F. J. Rotella, A. W. Schulke, P. Thiyagarajan, F. Troun, T. G. Worlton
(708) 972-4999/(FTS) 972-4999 **04-1**
$5,425,000

Operation and development of IPNS, a pulsed spallation neutron source for condensed matter research with neutron scattering techniques. The facility is equipped with ten instruments which are regularly scheduled for users, two instruments under construction and one beam tube which is for an instrument under development. 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 260 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., DuPont, IBM, Schlumberger-Doll, Amoco, British Petroleum) 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 was recently installed that increased the flux by a factor of 2.5.

45. APS Accelerator R&D
Y. Cho, J. Bridges, J. Cook, E. Crosbie, S. Kim, M. Knott, S. Kramer, R. Kustom, G. Mavrogenes, G. Nicholls, L. Teng, K. Thompson, L. Turner, R. Wehrle
(708) 972-6616/(FTS) 972-6616 **04-1**
$5,146,000

Further refinement of the accelerator and storage ring design of the Advanced Photon Source, research supporting development of a 7-GeV storage ring complex facilitating wide ranges of tunability of insertion devices, and capable of operating with 34 insertion device beamlines compared to 28 insertion device beamlines of 6 GeV design. Development of accelerator component prototypes to evaluate and refine performance characteristics. Evaluation of theoretical methods to predict accelerator physics performance parameters. Research on accelerator vacuum systems fabrication and cleaning processes. Facility Title I design activities began in FY 1989 and construction will be initiated in FY 1990 according to current estimates.

46. APS Beamline and Insertion Device R&D
G. K. Shenoy, E. E. Alp, G. A. Forster, A. Khounsary, S. H. Kim, D. M. Mills, R. K. Smither, E. Stefanski, P. J. Viccaro
(708) 972-5537/(FTS) 972-5537 **04-1**
$621,000

Design studies of the components of the insertion devices, beam line components, X-ray optics, and detectors suitable for 7-GeV Advanced Photon Source. Methodology to calculate the angular distributions and polarization of insertion device radiation. Design of a linear CCD/scintillation detector for X-ray range and readout procedures to perform time development studies. Design and construction of prototype insertion devices for experimentation at the Cornell Electron Storage Ring and at the National Synchrotron Light Source X-ray ring, to evaluate insertion device performance and to conduct feasibility experimentation.

Brookhaven National Laboratory

Upton, NY 11973
M. Blume - (516) 282-3735/(FTS) 666-3735

Metallurgy and Ceramics - 01

K. Lynn - (516) 282-3819/(FTS) 666-3819

47. First Principles Theory of High and Low Temperature Phases
J. W. Davenport, P. Allen (SUNY-Stony Brook), G. Fernando, H.-Q. Lin, G.-X. Qian, R. E. Watson, M. Weinert
(516) 282-3789/(FTS) 666-3789 **01-1**
$486,000

First principles molecular dynamics simulations using electronic structure calculations based on the density functional method to study liquids and large unit cell alloys and disordered metals. Also studies of semiconductor surfaces using molecular dynamics.

48. Structure and Properties of Surface Modified Materials and Interfaces
S. M. Heald, B. Nielsen, M. W. Ruckman
(516) 282-2861/(FTS) 666-2861 **01-1**
$514,000

Experimental studies of the fundamental factors which influence the microstructure and chemical bonding at interfaces 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. Structural and chemical characterization is carried out using glancing angle X-ray reflection and absorption, and positron annihilation along with standard techniques such as transmission electron microscopy and photoemission.

49. Mechanisms of Metal-Environment Interactions
H. S. Isaacs, A. J. Davenport
(516) 282-4516/(FTS) 666-4516 **01-2**
$424,000

Studies of the properties, formation, and breakdown of passive and anodically grown oxide films on metals and alloys. Structure and valency of surface oxides using EXAFS and XANES. Studies of the incorporation of corrosion-inhibiting anions and the mobility of these anions under existing high electric fields. Electronic and ionic conductivities of oxide films. Kinetics of the early stages of formation of oxide films. Breakdown of oxide films followed by localized corrosion. Propagation of voltage transients along metal surfaces. Dissolution kinetics of metals in highly concentrated electrolytes. Structure of the electrolytes, salt film formation, and electromigration.

50. Superconducting Materials
M. Suenaga, D. O. Welch
(516) 282-4516/(FTS) 666-3517 **01-3**
$1,093,000

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.

51. Basic Materials Science of Conductor Fabrication
M. Suenaga
(516) 282-3518/(FTS) 666-3518 **01-5**
$472,000

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 - (516) 282-3763/(FTS) 666-3763

52. Elementary Excitations and New Techniques
L. Passell, M. Elmiger, L. Rebelsky, S. M. Shapiro
(516) 282-3825/(FTS) 666-3825 02-1
$1,418,000

This program is directed to the study of elementary excitations in condensed matter and to the development of new neutron scattering techniques to further these investigations. Currently, experimental interest focuses on excitations in heavy fermion, mixed valent and paramagnetic systems, on magnetism in synthetic multilayers, and on the structures and dynamical response of adsorbed gas films. The objective in all these experiments is to obtain a better understanding of the fundamental interactions which determine the unique properties of these systems. In the area of new instrumentation, the reflection spectrometer has been installed on the High Flux Beam Reactor (HFBR) cold moderator beamline and tests made of its performance. It is expected to be in routine operation within the year. This, as well as other recently completed projects and such continuing projects as the United States-Japan (U.S.-Japan) collaborative research program, represent a significant expansion of the condensed matter research capability of the HFBR. Part of the effort in new instrument development will also contribute to the Advanced Neutron Source Project at Oak Ridge National Laboratory.

53. Magnetic and Structural Phase Transitions
G. Shirane, H. Chou, P. M. Gehring, H. Moudden, J. M. Tranquada
(516) 282-3732/(FTS) 666-3732 **02-1**
$1,159,000

The principal objective of this program is the fundamental study of phase transitions and magnetism by elastic and inelastic neutron scattering. At present, a concentrated effort directed towards the characterization and understanding of the high temperature superconductors complements work on a wide-range of other important systems. Within the area of phase transitions, measurements of both structural rearrangements and dynamical fluctuations in order parameters are applied to martensitic alloys as well as to the copper-oxide superconductors. The unique attributes of the neutron are exploited in both the static and dynamical studies of critical phenomena in magnetic materials. The primary interest is in the study of collective magnetic excitations and short-range correlations in a wide variety of magnetic materials. Recent activity involves substitutionally disordered magnetic materials, spin glasses, and low-dimensional systems. Antiferromagnetic correlations are proving to be especially important in the copper-oxide perovskite systems. The facilities at the High Flux Beam Reactor (HFBR) are operated as a Participating Research Team and are available to the outside scientific community. Scientists from academia, industry, and other national laboratories are encouraged to perform their experiments at Brookhaven.

54. Structural Characterization of Materials Using Powder Diffraction Techniques
D. E. Cox, J. Hriljac, K. G. Lynn, A. Moodenbaugh
(516) 282-3818/(FTS) 666-3818 **02-2**
$257,000

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.

55. Low Energy—Particle Investigations of Solids
K. G. Lynn, R. Mayer, J. Throwe, M. Weber
(516) 282-3710/(FTS) 666-3710 **02-2**
$949,000

Perfect and imperfect solids, solid and liquid interfaces and their surfaces are investigated 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, and Thermal Desorption Spectroscopy). These methods include two-dimensional angular correlation of annihilation radiation, positronium scattering, positron channeling and diffusion lengths, positron work functions, and 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, and 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. Improved modeling of positron implantation and diffusion in homogeneous and layered solids through Monte Carlo simulation is being developed to carry out quantitative depth profiling.

56. Experimental Research—X-ray Scattering
S. K. Sinha, L. D. Gibbs, G. Grubel, K. Huang, B. Ocko
(516) 282-3821/(FTS) 666-3821 **02-2**
$1,090,000

The objective of this program is to exploit the technique X-ray scattering, particularly synchrotron X-ray scattering, to study structure and magnetism in solids and complex fluids. Emphasis is given to studies of the structure of surfaces, interfaces, and thin films utilizing a UHV X-ray scattering chamber and special X-ray cells for studying scattering from solid/liquid and liquid/vapor interfaces. Magnetic structure is probed via magnetic X-ray scattering, particularly resonant magnetic scattering. Polarization analysis has also been used to separate the spin and orbital magnetization densities in solids.

57. Theoretical Research
J. W. Davenport, P. Bak, K. Chen, V. J. Emery, O. Piro, R. E. Watson, M. Weinert
(516) 282-3789/(FTS) 666-3789 **02-3**
$898,000

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, self organized criticality, 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.

58. Surface Physics Research
M. Strongin, P. D. Johnson, C. L. Lin, S. L. Qui, A. Viescas
(516) 282-3763/(FTS) 666-3763 **02-5**
$937,000

Various surface sensitive techniques are used to study the geometrical and electronic properties of surfaces and interfaces. These techniques include LEED, Auger 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) catalytic properties of metal overylayers; (c) core level photoemission and near edge studies of the high T_c superconductors; (d) surface metallurgy and surface compounds; (e) photoemission studies of low temperature oxidation; (f) studies of metastable species formed in low temperature reactions and (g) studies of surface magnetism in thin films and the effect of adsorption on surface magnetism.

Materials Chemistry - 03
N. Sutin - (516) 282-4301/(FTS) 666-4301

59. Neutron Scattering
J. Z. Larese
(516) 282-4349/(FTS) 666-4349 **03-1**
$455,000

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 the structure of thin films on surfaces, wetting and surface melting, martensitic alloys, Rayleigh-Benard convection in $^3He/^4He$ mixtures and oxymetallates. 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 elastic, absorptive, and inelastic neutron techniques presents 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.

60. Synthesis and Structures of New Conducting Polymers
T. A. Skotheim
(516) 282-4490/(FTS) 666-4490 **03-2**
$461,000

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, CUNY, University of Lowell and Massachusetts Institute of Technology.

Facility Operations - 04
M. Brooks - (516) 282-4061

61. High Flux Beam Reactor —Operations
M. H. Brooks, W. Brynda, J. Detweiler, O. Jacobi, J. Junker, V. Lettieri, J. Petro, T. Prach, R. Reyer, D. C. Rorer, P. Tichler
(516) 282-4061/(FTS) 666-4061 **04-1**
$14,300,000

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.

62. National Synchrotron Light Source, Operations and Development
M. Knotek, A. M. Fauchet, J. Galayda, R. Garrett, J. Godel, J. Hastings, R. Heese, H. Hsieh, R. Klaffky, S. Krinsky, C. Pellegrini, W. Thomlinson, G. Vignola
(516) 282-4966/(FTS) 666-4966 **04-1**
$13,430,000

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 beamlines 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.

Idaho National Engineering Laboratory
P. O. Box 1625
Idaho Falls, ID 83415
D. W. Keefer - (208) 526-8003

63. Entrapped Helium in Rapidly Solidified Material
R. N. Wright
(FTS) 583-6127 **01-5**
$130,000

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 - (217) 333-1370

Metallurgy & Ceramics - 01
H. K. Birnbaum - (217) 333-1370

64. Transport Processes on Localized Corrosion
R. C. Alkire
(217) 333-3640 **01-1**
$131,000

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.

65. Defect, Diffusion, and Non-Equilibrium Processing Of Materials
R. S. Averback
(217) 333-4302 **01-1**
$278,000

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.

66. Center for Microanalysis of Materials
J. A. Eades, C. Loxton, J. Woodhouse
(217) 333-8396 **01-1**
$113,000

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.

67. Microanalysis of Defects and Interfaces
J. A. Eades
(217) 333-8396 **01-1**
$113,000

Defects, interfaces, 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.

68. Growth and Transport at Metal and Semiconductor Interfaces
G. Ehrlich
(217) 333-6448 **01-1**
$198,000

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.

69. Local Strain Determinations at Interfaces in Metals and Semiconductors
H. L. Fraser
(217) 333-1975 **01-1**
$117,000

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.

70. Chemistry of New Transition Metal Ceramic Compounds Synthesized by MOCVD
G. S. Girolami
(217) 333-2729 **01-1**
$142,000

Synthesis of thin film ceramics by chemical vapor deposition method. Studies of the chemistry of precursor compounds at solid surfaces. Preparation 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.

71. Crystal Growth and Physical Properties of Single Crystal Metastable Semiconductors
J. E. Greene
(217) 333-0747 **01-1**
$209,000

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-V2 chalcopyrite systems.

72. Processing and Microstructure of Complex Ceramic Systems
A. Zangvil
(217) 333-6829 **01-1**
$187,000

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.

73. Mechanisms of Environmentally Induced Embrittlement
C. J. Altstetter
(217) 333-4985 **01-2**
$95,000

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.

74. Solute Effects on Mechanical Properties of Grain Boundaries
H. K. Birnbaum
(217) 333-1370 **01-2**
$220,000

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.

75. Council On Materials Science
C. P. Flynn
(217) 333-1370 **01-2**
$125,000

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.

76. High Temperature Toughening Methods in Composite Ceramics
W. T. Kriven
(217) 333-5258 **01-2**
$68,000

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.

77. Mechanical Properties of Intermetallic Compounds
C. Loxton, I. M. Robertson
(217) 333-0386 **01-2**
$149,000

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.

78. The Role of Deformation Mechanisms in Multiaxial Deformation and Cyclic Fatigue
D. F. Socie
(217) 333-7630 **01-2**
$78,000

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, multiaxial, and fatigue conditions.

79. Micromechanisms of Fracture
J. F. Stubbins
(217) 333-6474 **01-2**
$50,000

Micromechanisms of failure at elevated temperatures under creep, fatigue and aggressive environmental conditions. Role of oxide films on crack initiation and propagation. Microstructural examination of regions in front of cracks and of the dislocation structures are related to micromechanics of failure. Crack propagation kinetics in ceramics at high temperatures and in aggressive atmospheres. Subcritical crack growth in ceramics.

80. Structure and Kinetics of Ordering Transformations in Metal Alloys and Silicide Thin Films
H. Chen
(217) 333-7636 **01-3**
$100,000

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.

81. Materials Chemistry of Oxides Ceramics
W. F. Klemperer
(217) 333-2995 **01-3**
$197,000

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.

82. Synthesis and Properties of Dielectric Solids
D. A. Payne
(217) 333-2937 **01-3**
$261,000

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.

83. Atomic Scale Mechanisms of Vapor Phase Crystal Growth
A. Rockett
(217) 333-0417 **01-3**
$97,000

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.

84. Processing of Monodisperse Ceramic Powders
C. Zukoski
(217) 333-7379 **01-3**
$221,000

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.

85. Ultrasonic Studies of Radiation Effects
A. V. Granato
(217) 333-2639 **01-4**
$24,000

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.

86. Radiation Damage in Metals and Semiconductors
I. M. Robertson
(217) 333-6776 01-4
$67,000

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.

Solid State Physics - 02
H. Zabel - (217) 333-2514

87. Low Temperature Studies of Defects in Solids
A. C. Anderson
(217) 333-2866 02-2
$102,000

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.

88. Synthesis and Properties of Organometallic Liquid Crystalline Polymers
T. L. Brown
(217) 244-1176 02-2
$23,000

Synthetic routes to liquid crystal polymers containing transition metal organometallic functional groups are being explored. These groups are chosen to have special chromophoric, electric or magnetic properties.

89. Electronic Properties of Semiconductor Surfaces and Interfaces
T.-C. Chiang
(217) 333-2593 02-2
$147,000

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.

90. Theory of Solids, Surfaces and Heterostructures
R. M. Martin
(217) 333-4229 02-2
$98,000

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.

91. Investigations of Crystal Growth by Molecular Beam Epitaxy
H. Morkoc, C. P. Flynn
(217) 333-0722 02-2
$238,000

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.

92. Organometallic Nonlinear Materials
T. B. Rauchfuss
(217) 333-7355 02-2
$58,000

A research program for the synthesis of organometallic polymers. The program emphasizes fundamental synthetic chemistry as it applies to the design of monomers suited for polymerization. Solids containing dynamic metal-metal bonds, i.e., mobile charge density waves. Syntheses of metal clusters contianing reactive ester groups will be developed for the applications to organometallic polyesters. The reactivity inherent in main group vertices of metal clusters will be used to generate clusters-of-clusters. Synthetic studies will focus on charge transfer salts containing organometallic donors and acceptors.

93. Properties of Crystalline Condensed Gases
R. O. Simmons
(217) 333-4170 02-2
$175,000

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.

94. Nuclear Magnetic Resonance in Solids
C. P. Slichter
(217) 333-3834 02-2
$209,000

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.

95. Electroactive and Non-Linear Optical Polymers
S. I. Stupp
(217) 333-4436 02-2
$68,000

Synthesis and physical property determination of self ordering chiral polymers that order in response to external fields. Fields of interest are electric, stress and flow, and optical responses. Properties of interest in these polymers are ferroelectricity, ferromagnetism and non-linear optical properties.

96. Metalloporphyrins as Field Responsive Materials
K. S. Suslick
(217) 333-2794 02-2
$22,000

The synthesis and characterization of porphyrinic materials with ferroelectric and non-linear optical properties are being studied. Metalloporphyrin polymers, linked by direct metal-porphyrin chains via lanthanide metals or bridging, non-symmetric bifunctional ligands are being developed. Asymmetric assemblies with large molecular species having large dipole moments are being studied.

97. Carrier Transport in Quantum Wells Picosecond Imaging
J. P. Wolfe
(217) 333-2374 02-2
$106,000

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.

98. Structure and Dynamics of Surfaces, Interfaces and Heterostructures
H. Zabel
(217) 333-2514 02-2
$128,000

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.

Materials Chemistry - 03
H. Zabel - (217) 333-2514

99. Pressure Tuning Spectroscopy
H. G. Drickamer
(217) 333-0025 03-1
$163,000

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.

100. Advanced Microstructures for Photochemical and Electrochemical Energy Conversion
L. R. Faulkner
(217) 333-8306 03-1
$86,000

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.

101. Surface Studies of Boundary Layer Films
A. J. Gellman
(217) 244-5810 **03-1**
$77,000

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.

102. Optical Spectroscopy of Surface Processes in this Film Deposition
E. G. Seebauer
(217) 333-4402 **03-1**
$49,000

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.

Lawrence Berkeley Laboratory

1 Cyclotron Road
Berkeley, CA 94720
N. E. Phillips - (415) 486-6063/(FTS) 451-6063

Metallurgy and Ceramics - 01

N. E. Phillips - (415) 486-6063/(FTS) 451-6063

103. CAM Ceramic Processing Science Program
Lutgard C. De Jonghe
(415) 486-6138/(FTS) 451-6138 **01-1**
$975,000

The CAM Ceramic Processing Science Program has three linked objectives: the development of predictive, quantitative theories of densification and microstructure development in heterogeneous powder compacts, the application of these theories to produce advanced structural ceramics with improved high temperature performance, and the evaluation of the mechanical properties of these ceramics. It develops models and means for initial powder compact structural control including the production and use of coated powders; it examines the microstructural evolution and control during densification in relation to interface properties; it produces particulate ceramic composites based on SiC, and it tests mechanical properties of such ceramics in particular high temperature creep and fatigue.

104. In Situ Investigations of Gas-Solid Reactions by Electron Microscopy
J. W. Evans
(415) 642-3807/(FTS) 451-3807 **01-1**
$80,000

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.

105. Structure And Properties of Transformation Interfaces
R. Gronsky
(415) 486-5674/(FTS) 451-5674 **01-1**
$174,000

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.

106. CAM Structural Materials Program
J. W. Morris, Jr.
(FTS) 451-6482 **01-1**
$550,000

This CAM program focuses on advanced structural materials of interestto 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. De-Jonghe), 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.

107. Microstructure, Properties, Alloy Design: Inorganic Materials
G. Thomas
(415) 486-5656/(FTS) 451-5656 01-1
$495,000

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.

108. National Center for Electron Microscopy
G. Thomas, R. Gronsky, K. H. Westmacott
(516) 486-5656/(FTS) 451-5656 01-1
$1,545,000

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.

109. Solid-State Phase Transformation Mechanisms
K. H. Westmacott
(415) 486-5663/(FTS) 451-5663 01-1
$174,000

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.

110. Local Atomic Configurations in Solid Solutions
D. de Fontaine
(415) 642-8177/(FTS) 451-8177 01-1
$124,000

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.

111. Alloy Theory
D. de Fontaine
(415) 642-8177 01-1
$186,000

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.

112. Ceramic Interfaces
A. M. Glaeser
(415) 642-3821/(FTS) 451-3821 01-3
$138,000

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 grain boundaries in sapphire/alumina 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.

113. CAM Electronic Materials Program
E. Haller, R. M. Cannon, Jr., J. W. Morris, J. Washburn
(415) 642-5294/(FTS) 451-5294 **01-3**
$1,000,000

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).

114. High-Temperature Reactions
A. W. Searcy
(415) 642-5900/(FTS) 451-5900 **01-3**
$230,000

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.

Solid State Physics - 02
N. E. Phillips - (415) 486-6063/(FTS) 451-6063

115. Center for X-ray Optics
D. Attwood
(415) 642-4463/(FTS) 451-4463 **02-2**
$1,563,000

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.

116. Superconductivity, Superconducting Devices, and 1/F Noise
J. Clarke
(415) 642-3069/(FTS) 451-3069 **02-2**
$231,000

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.

117. Nonlinear Excitations in Solid-State Systems
C. D. Jeffries
(415) 642-3382/(FTS) 451-3382 **02-2**
$153,000

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.

118. Interfacial Materials and Processes
J. D. Porter
(415) 642-7236/(FTS) 451-7236 **02-2**
$40,000

Ultralow-defect single-crystal metal surfaces prepared and characterized in situ, and used as de facto standards for the development of new techniques. High-resolution structural and spectroscopic methods to be developed are simultaneous atomic force and scanning tunneling microscopy (AFM/STM), which will allow deconvolution of topographic (structural) and electronic (bonding) effects with atomic resolution, and photoelectron tunneling spectroscopy (PTS), in which a macroscopic metal/liquid/metal tunneling junction is used with a high-brightness photon source to probe valence and core-level electronic structure at the interface.

119. Far-Infrared Spectroscopy
P. L. Richards
(415) 642-3027/(FTS) 451-3027 **02-2**
$208,000

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.

120. Studies of the Metal/Solution Interface with X-rays
P. N. Ross
(415) 486-6226/(FTS) 451-6226 **02-2**
$50,000

Development of a new method to determine the in situ structure at metal/solution interfaces using total reflection of X-rays from metal surfaces at glancing incidence and analysis of Bragg reflection parallel and perpendicular to the reflecting plane to obtain complete structural characterization of the interfacial region. Proof-of-principle experiments conducted on the 54-pole wiggler beamline at SSRL. Initial experiments directed towards the study of the electrolytic growth of thin (100 nm) metal epilayers and the elucidation of dislocation creation and propagation, and the study of the electrolytic reconstruction of metal surfaces and the understanding of solvated ion-metal interaction that causes this phenomenon (related to the more familiar reconstruction of the (100) faces of Au, Pt, and Ir in UHV). Future experiments planned for the Advanced Light Source, where the unique high brightness of this source is very advantageous for the glancing incidence geometry in these experiments.

121. Experimental Solid-State Physics and Quantum Electronics
Y. R. Shen
(415) 642-4856/(FTS) 451-4856 **02-2**
$232,000

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.

122. Time-Resolved Spectroscopies in Solids
P. Y. Yu
(415) 642-8087/(FTS) 451-8087 02-2
$107,000

The main objective of this project is to utilize picosecond and subpicosecond 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.

123. Quantum Theory of Materials
M. L. Cohen, L. M. Falicov, S. G. Louie
(415) 642-4753/(FTS) 451-4753 02-3
$245,000

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.

124. CAM High-Tc Superconductivity Program
N. E. Phillips, P. Berdahl, J. Clarke, L. C. DeJonghe, R. Gronsky
(415) 486-6382/(FTS) 451-6382 02-5
$500,000

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.

Materials Chemistry - 03
N. E. Phillips - (415) 486-6063/(FTS) 451-6063

125. Low-Temperature Properties of Materials
N. E. Phillips
(415) 486-6063/(FTS) 451-6063 03-1
$145,000

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.

126. CAM Polymers and Composites Program
M. M. Denn
(415) 642-0176/(FTS) 451-0176 03-2
$900,000

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.

127. Electrochemical Phase Boundaries
R. H. Muller
(415) 486-6079/(FTS) 451-6079 03-2
$124,000

Nucleation and growth processes in the electrocrystallization of metals from aqueous media from first atomic layers to macroscopic thicknesses. Effect of adsorbed molecules on early stages of film formation. Development and use of in situ techniques for following composition, structure, and microtopography during film formation: scanning tunneling microscopy, Raman spectroscopy, spectroscopic ellipometry. Comparison of measurements with predictions of theoretical models that consider kinetic factors, convective diffusion of ions and molecules, and the electric field at the interface.

128. Electrochemical Processes
C. W. Tobias
(415) 642-3764/(FTS) 451-3764 03-2
$74,000

Investigation of novel methods for reducing mass-transfer resistance in high-rate electrolysis, including in electroforming, and in electrosynthesis. Effects of suspended inert particles in flowing electrolytes, on transport rates, and on current distribution are measured over broad ranges of process variables; theoretical models are advanced for the interpretation of mechanisms. Novel approaches are explored, and the relevant theoretical framework is established for the control of composition and phase structure in the electrodeposition of alloys.

129. High-Temperature Thermodynamics
L. Brewer
(415) 486-5946/(FTS) 451-5946 03-3
$129,000

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.

130. Chemistry and Materials Problems in Energy Production Technologies
D. R. Olander
(415) 642-7055/(FTS) 451-7055 03-3
$221,000

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 U02. 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.

131. Nuclear Magnetic Resonance
A. Pines
(415) 486-6097/(FTS) 451-6097 **03-3**
$700,000

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 systems such 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.

132. CAM Surface Science and Catalysis Program
G. A. Somorjai
(415) 642-4053/(FTS) 451-4053 **03-3**
$1,500,000

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 metalpolymer (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).

133. Synthesis Of Novel Solids
A. M. Stacy
(415) 642-3450/(FTS) 451-3450 **03-3**
$135,000

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.

Accelerator and Fusion Research Division
K. Berkner - (415) 486-5501/(FTS) 451-5501

134. 1-2 GeV Synchrotron Light Source R&D
J. N. Marx
(415) 486-5244/(FTS) 451-5244 **04-1**
$1,873,000

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 Lab

P. O. Box 808
Livermore, CA 94550
T. Sugihara - (415) 423-8351/(FTS) 543-8351

135. Systematics of Phase Transfer in Metallic Alloys
L. Tanner
(415) 423-2653/(FTS) 543-2653 **01-1**
$290,000

Investigations of the systematics of solid-to-solid and liquid-to-solid phase transformations in metallic alloys. Thermal, mechanical or irradiation treatments are being used to transform one crystalline phase to another or to the amorphous or metallic glass state. Characterization of microstructures by optical and conventional and high-resolution transmission electron microscopy, as well as X-ray and electron diffraction. Correlation of results with current thermodynamic and kinetic models for diffusional (replacive) and non-diffusional (displacive) transformations, solidification and solid-state amorphization. Theoretical modeling of alloy phase stability and phase transformation modes are being carried out using a combination of quantum mechanics and statistical mechanics methods.

136. Optical Materials Research
L. L. Chase, H. Lee, S. Payne, N. Winter
(415) 423-6151/(FTS) 543-6151 **02-2**
$870,000

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. Coherence properties of optical excitations are investigated with subpicosecond time resolution. 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.

137. Effect of Impurities, Flaws and Inclusions on Adhesion and Bonding at Internal Interfaces
W. E. King, M. I. Baskes, A. Gonis, E. Sowa
(415) 423-6547/(FTS) 543-6547 **01-2**
$250,000

Experimental and theoretical investigations of the effects of impurities, flaws and inclusions on adhesion and bonding at internal interfaces. Specifically, structure and properties of gain boundaries in Nb. Ab initio electronic structure calculations using the real-space multiple-scattering theory. Interface structure calculations using the embedded atom method. Bicrystals for experimental studies fabricated using ultra high vacuum diffusion bonding. Determination of interface atomic structure using high resolution electron microscopy. Property measurements include grain boundary energy and grain boundary diffusion.

Los Alamos National Laboratory

P. O. Box 1663
Los Alamos, NM 87545
R. J. Jensen - (505) 667-1600/(FTS) 843-1600

Metallurgy and Ceramics - 01

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

138. Irradiation-Induced Metastable Structures in Ceramics and High-Temperature Superconductors
F. W. Clinard, Jr.
(505) 667-5102/(FTS) 843-5102 **01-4**
$490,000

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 nonirradiation-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.

139. Interfacial and Radiation Effects in Structural and Superconducting Ceramics
T. E. Mitchell, F. W. Clinard, A. L. Graham, J. J. Petrovic
(505) 667-0938/(FTS) 843-0938 **01-5**
$595,000

Interface effects in structural ceramic composites. Synthesis of Si_3N_4, SiC and Al_2O_3 ceramics with VLS SiC whiskers. Interface modification. Characterization by high resolution an analytical electron microscopy. Interface adhesion and crack propagation in ceramic composites. Modeling of stress distribution and crack propagation by finite element codes. Irradiation-induced structures produced in high temperature superconductors by electronic excitation, ion bombardment and neutron radiation. Characterization by HREM, AEM stored energy, electrical and magnetic property measurements. The role of irradiation in strength, fracture and interfacial properties of structural ceramics.

140. Structural Ceramics
D. S. Phillips, T. N. Taylor, K. C. Ott, P. D. Shalek, J. L. Craig
(505) 667-5128/(FTS) 843-5128 **01-5**
$372,000

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.

141. Metastable Phases and Microstructures
R. B. Schwarz, T. E. Mitchell
(505) 667-8454/(FTS) 843-8454 **01-5**
$249,000

Fundamental research on the theory, synthesis, microstructures, and properties of materials with metastable phases. The research includes: (a) the synthesis of amorphous alloys by mechanical alloying and interdiffusion; (b) the study of phase equilibria and transformation kinetics in solid-state transformations; (c) the characterization of microstructures at atomic level of resolution developed during solid-state transformations; (d) the relationship between microstructures and properties in metastable and transformed materials; (e) the application to material properties such as mechanical strength, magnetic behavior, catalysis, and superconductivity; and (f) the study of the microstructure, twin morphology, and dislocation structure in high T_c pervoskites and its relation to transport properties.

142. Mechanical Properties
M. G. Stout, U. F. Kocks
(505) 667-4665/(FTS) 843-4665 **01-5**
$520,000

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes, Bauschinger effects. Characteristics of mechanisms controlling the large strain deformation of aluminum, nickel, iron, copper, brass, sub-structural 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.

Solid State Physics - 02
D. M. Parkin - (505) 667-8455/(FTS) 843-8455

143. Condensed Matter Research with the LANSCE Facility
R. Pynn
(505) 667-6069/(FTS) 843-6069 **02-1**
$1,947,000

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 in quantum solids and liquids, molecular vibrations, surface-absorbed 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.

144. Correlated Electrons in Metals
Z. Fisk, A. Arko, J. D. Thompson
(505) 665-0892/(FTS) 843-0892 **02-2**
$244,000

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 the exotic properties in heavy Fermion, high T_c oxide and other marrow-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.

145. Materials Under Extreme Conditions
D. Schiferl, R. LeSar, J. W. Shaver
(505) 665-3150/(FTS) 843-3150 **02-2**
$234,000

Studies of phase transformations, crystal structures, changes in bonding, and thermodynamics of simple molecular systems at high pressures (up to 1 Mbar) and extreme temperatures (10-1800 K). Develop theories of phase transformations, structural behavior, and chemical reactor kinetics. Experimental techniques include laser Raman spectroscopy, uv-vis-ir spectroscopy, impulse-stimulated Brillouin scattering and X-ray diffraction on samples in diamond anvil cells. Develop high-temperature diamond-anvil cell technology, including refractory metal alloys for cell components. Theoretical techniques include molecular dynamics and Monte Carlo simulations, electronic structure calculations, and analytical methods.

146. Investigations of Superconductors with High Critical Temperatures
J. L. Smith, K. C. Ott, J. D. Thompson
(505) 667-4476/(FTS) 843-4476 **02-5**
$500,000

Effort is focused on developing fundamental understandings of the dependences of T_c and J_c on the composition, processing, and underlying physics of high transition temperature superconducting oxides. At the heart of superconductivity applications is the requirement of large, dissipationless current carrying capacity. Activities directed toward achieving this goal include chemically modifying oxide superconductors with dopants that either scavenge insulating materials ("weak-links") from grain boundaries, or that provide flux pinning sites within crystallites. The materials studied include $Ba_{1-x}K_xBiO_3$, RE-123, both hole- and electron-doped $RE_{2-x}M_xCuO_4$, and the layered Bi and Tl materials containing multiple CuO_2 layers. Research on new materials is included. This project is coordinated with the Los Alamos Superconductivity Pilot Center.

147. Thermal Physics
G. W. Swift, R. Ecke
(505) 665-0640/(FTS) 843-0640 **02-5**
$276,000

Thermal convection experiments in dilute solutions of ^3He in superfluid ^4He near 1 K and in rotating water at room temperature: steady and oscillatory, nonlinear dynamics and chaos, optical shadowgraph imaging. Experimental and theoretical studies of novel engines: acoustic engines (both heat pumps and prime movers) using liquids, gases, and superfluids; acoustic turbulence; liquid propylene Stirling engine: regenerators, heat exchanges, mechanicals, seals. Superfluid liquid ^3He: A to B phase transition dynamics experiments.

Materials Chemistry - 03

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

148. Originating Super-Strong Liquid-Crystalline Polymers
F. Dowell, B. C. Benicewicz, R. Liepins
(505) 667-8765/(FTS) 843-8765 **03-2**
$524,000

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. Progress has been made in the origination of theories for LCPs and 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.

149. Low-Dimensional Mixed-Valence Solids and Conducting Polymers
B. I. Swanson, M. Aldissi, A. R. Bishop
(505) 667-5814/(FTS) 843-5814 **03-2**
$270,000

This is a theoretical and experimental effort to characterize the model low-dimensional mixed-valence solids as they are tuned, with pressure and chemistry, from a charge-density-wave (CDW) ground state towards a valence delocalized state. The systems of interest are comprised of alternating transition metal complexes and bridging groups that form linear chains with strong electron-electron and electron-phonon coupling down the chain axis. The ground and local gap states (polarons, bipolarons, excitons, and kinks) are characterized using structural, spectroscopic and transport measurements and this information is correlated with theoretical predictions. The theoretical effort includes quantum chemistry, band structure, and many-body methods to span from the isolated transition metal complexes to the extended interactions present in the solid state. It includes investigation of conductivity-structure-property relations in conducting polymers.

150. LANSCE Operations Support, Spectrometer Development, and User Support
R. Pynn
(505) 667-6069/(FTS) 843-6069 **04-1**
$3,250,000

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 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 reflectrometer with a polarized-neutron option; and a back-scattering spectrometer with a resolution of 10 eV or better. A national user program required 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 Associated Universities
Oak Ridge, TN 37831
A. Wohlpart - (615) 576-3000/(FTS) 626-3255

151. Oak Ridge Synchrotron Organization for Advanced Research
T. A. Habenschuss, R. DeAngelis, S. Moss, Jr., C. J. Sparks, R. Young
(615) 576-5614/(FTS) 626-5614 **01-1**
$113,000

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 resolutionsof delta E/E = 2 x 10-4. One Oak RidgeAssociated 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.

152. Shared Research Equipment Program (SHARE)
E. A. Kenik, N. Evans
(615) 574-4427/(FTS) 624-4427 **01-1**
$95,000

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 dis- persive 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 Vande Graaff accelerators for Rutherford backscattering and nuclear reaction techniques.

Oak Ridge National Laboratory

P. O. Box 2008
Oak Ridge, TN 37831-6117
B. R. Appleton - (615) 574-4321/(FTS) 624-4321

Metallurgy and Ceramics - 01

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

153. Microscopy and Microanalysis
J. Bentley, D. C. Joy, E. A. Kenik, M. K. Miller
(615) 574-5067/(FTS) 624-5067 **01-1**
$858,000

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.

154. Theoretical Studies of Metals and Alloys
W. H. Butler, C. L. Fu, G. S. Painter,
G. M. Stocks, N. Wright
(615) 574-4845/(FTS) 624-4845 **01-1**
$845,000

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.

155. X-ray Research Using Synchrotron Radiation
C. J. Sparks, Jr., G. E. Ice, E. D. Specht
(615) 574-6996/(FTS) 624-6996 01-1
$488,000

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, 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.

156. Radiation Effects
L. K. Mansur, R. A. Buhl, R. E. Clausing,
K. Farrell, Jr., L. Heatherly, E. H. Lee,
M. B. Lewis, D. Pedraza, R. E. Stoller
(615) 574-4797/(FTS) 624-4797 **01-4**
$1,220,000

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, $MgAl_2O_4$.

157. Toughening and Related Processing Mechanisms in Ceramics
P. F. Becher, K. B. Alexander, A. Bleier, C.-H. Hsueh
(615) 574-5157/(FTS) 624-5157 **01-5**
$908,000

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 macro-scopic 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).

158. Fundamentals of Welding and Joining
S. A. David, J. M. Vitek
(615) 574-4804/(FTS) 624-4804 **01-5**
$515,000

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.

159. High Temperature Alloy Design
C. T. Liu, E. P. George, J. A. Horton, W. C. Oliver, W. D. Porter, J. H. Schneibel, M. H. Yoo
(615) 574-4459/(FTS) 624-4459 **01-5**
$1,232,000

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.

160. Structure and Properties of Surfaces and Interfaces
C. J. McHargue, M. B. Lewis, F. A. List, R. A. McKee, P. S. Sklad
(615) 574-4344/(FTS) 624-4344 **01-5**
$947,000

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 interfaces, stress relaxation and dissipation. Adherence of oxide and metal films. Ion beam mixing and amorphization of multi-layer metallic alloys and ceramics. MBE growth of layered ceramics.

Solid State Physics - 02

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

161. Interatomic Interactions in Condensed Systems

R. M. Moon, J. W. Cable, J. Fernandex-Baca, C. M. Malone, H. A. Mook, R. M. Nicklow, H. G. Smith
(615) 574-5234/(FTS) 624-5234 02-1
$790,000

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, magnetic excitations in amorphous systems, phase transitions, nuclear spin ordering, momentum distributions in quantum fluids. New research directions will include more emphasis on materials properties under extreme environments of high pressures, high temperatures, or ultralow temperatures.

162. Properties of Defects, Superconductors, and Hydrides

R. M. Moon, H. R. Child, J. B. Hayter, ook. H. A. , S. Spooner, G. D. Wignall
(615) 574-5234/(FTS) 624-5234 02-1
$741,000

Elastic, inelastic, and small-angle scattering of neutrons by superconductors and metal hydrides, phase transitions, heavy fermion superconductors, high-T_c superconductors and reentrant superconductors, small-angle neutron scattering from ferrofluids, micelles under shear, polymers and polymer blends, metal alloys, liquid crystals and biological systems, kinetics of first-order phase transitions.

163. 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
(615) 574-5240/(FTS) 624-5240 02-1
$754,000

Neutron scattering facilities are available to outside scientists through the 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 inbones. New facilities include a high-resolution powder diffractometer and a four-circle single-crystal diffractometer with a cryostat for low-temprature crystallography studies.

164. Properties of Advanced Ceramics

J. B. Bates, Y. Chen, N. J. Dudney, G. R. Gruzalski, F. A. Modine, J. C. Wang
(615) 574-6280/(FTS) 624-6280 02-2
$925,000

Physical and chemical properties of advanced ceramics including single-phase and composite materials as well as thin-film, layered, and surface-modified structures prepared by novel techniques. Materials investigated include metal oxides, composites with metal oxides; thin films of amorphous and crystalline ionic and mixed ionic-electronic conductors; bulk and thin-film optical materials such as zinc oxide and rare-earth doped orthophosphates. Films prepared by magnetron sputtering, ion beam sputtering, electron beam evaporation, and plasma polymerization. Studies include ion transport in bulk compositeand thin-film electrolytes, electrodes, and electrode-electrolyte interfaces; electrical, dielectric, and optical properties of bulk and thin-film materials. Techniques include impedance spectroscopy, transient signal analysis, Raman scattering, infrared reflectance-absorption, scanning electron microscopy, model calculations, and computer simulation.

165. Synthesis and Properties of Novel Materials

L. A. Boatner, M. M. Abraham, C. B. Finch, H. E. Harmon, J. O. Ramey, B. C. Sales
(615) 574-5492/(FTS) 624-5492 02-2
$1,150,000

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 implantation and ion channeling, optical absorption, high performance liquid chromatography, EPR, and neutron scattering; application of materials science 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; 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, rapid solidification and microstructures. 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 implantation and ion channeling, optical absorption, high performance liquid chromatography, EPR, and neutron scattering; application of materials science 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; 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, rapid solidification and microstructures.

166. Semiconductor Physics and Photophysical Processes of Solar Energy Conversion
D. H. Lowndes, D. J. Eres, D. B. Geohegan, G. E. Jellison, D. N. Mashburn, D. P. Norton, S. J. Pennycook, R. F. Wood
(615) 574-6306/(FTS) 624-6306 **02-2**
$925,000

Time-resolved reflectivity, transmissivity, and ellipsometric measurements, time-resolved transient electrical conductivity, light-assisted chemical vapor deposition of thin films, modulated layered structures, 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 infra-red 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.

167. Physical Properties of Superconductors
S. T. Sekula, D. K. Christen, H. R. Kerchner, C. E. Klabunde, J. R. Thompson
(615) 574-6271/(FTS) 624-6271 **02-2**
$405,000

Physical properties of superconductors, particularly high T_c materials, in various thin-film, single-crystal, sintered, and composite forms. Configurations of thin films include epitaxial, mixed epitaxial, and polycrystalline layers on single and polycrystalline substrates of several compounds, including $SrTiO_3$, $KTaO_3$, and other perovskites. Also, RF and DC sputtering are employed for preparation of precursor films. Highly aligned composites with dispersed particles of rare-earth and thallium-based superconducting compounds are fabricated, in addition to normal metal-superconductor composites. Investigations include the critical current density, normal state and flux flow resistivity, flux pinning and flux creep, upper and lower critical fields, magnetic penetration depth, magnetic susceptibility and magnetization. Techniques and facilities include electrical transport with variable orientation of applied magnetic fields up to 8 tesla, dc magnetization using a SQUID-based instrument with 5-tesla capability and vibrating sample magnetometry to 9 Torr ac magnetic response, and ion irradiation.

168. Small-Angle X-ray Scattering
G. D. Wignall, J. S. Lin, S. Spooner
(615) 574-5237/(FTS) 624-5237 **02-2**
$165,000

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).

169. Theory of Condensed Matter
J. F. Cooke, J. H. Barrett, H. L. Davis, R. Fishman, K. Flensberg, M. S. Jonon, T. Kaplan, S. H. Liu, G. D. Mahan, G. D. Mostoller, O. S. Oen, S. Pettersson, M. Rasolt, M. T. Robinson, J. C. Wang, R. F. Wood
(615) 574-5787/(FTS) 624-5787 **02-3**
$1,179,000

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, self-organized critical systems, basic mechanism and phenomenology of high-temperature superconductivity.

170. Structural Properties of Materials—X-ray Diffraction
B. C. Larson, J. D. Budai, M. D. Galloway, J. Z. Tischler
(615) 574-5506/(FTS) 624-5506 02-4
$551,000

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 semiconductor, defects associated with laser and thermal processing of pure and ion-implanted semiconductors, grain boundaries in semiconductors, microstructural characterization of high-temperature superconductors, solid-phase recrystallization in semiconductors, anisotropic elastic theory of dislocation loops, calculation of diffuse scattering from dislocation loops and solute precipitates, energy-resolved X-ray scattering, quasi-elastic scattering, phase transformations, theory of scattering of X-rays from defects in solids.

171. Electron Microscopy of Materials
S. Pennycook, M. F. Chisholm, D. Jesson
(615) 574-5504/(FTS) 624-5504 02-4
$550,000

Microstructure and properties of defects in solids, transmission electron microscopy, scanning transmission electron microscopy, atomic resolution microstructural characterization of semiconductors, superconductors and thin films with chemical specificity, enhanced diffusion in semiconductors, defects associated with laser and thermal processing of pure and ion-implanted semiconductors, grain boundaries in semiconductors and superconductors, high-resolution atomic imaging of defects, direct imaging and microscopic lattice location of dopants in semiconductors, solid-phase recrystallization in semiconductors, computer simulation of electron microscopy images, development of atomic resolution analytical techniques of electron microscopy, phase transformations, theory of scattering of electrons from defects in solids.

172. Research and Development—Isotope Research Materials Preparation
W. S. Aaron, J. R. Gibson, M. Petek
(615) 574-5916/(FTS) 624-5916 02-5
$208,000

Research and development of preparative techniques applicable to isotopic materials. Stable and radioactive enriched 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, ion beam and planar magnetron), rolling, electrodeposition, molecular plating, liquid phase and conventional sintering, hot pressing, reduction/distillation, 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, in situ film thickness monitoring, and sophisticated radiation counting methods.

173. Surface Modification and Characterization Facility and Collaborative Research Center
C. W. White, J. L. Moore, J. B. Roberto, III, O. E. Schow, T. P. Sjoreen, D. K. Thomas, S. P. Withrow
(615) 574-6295/(FTS) 624-6295 02-5
$1,154,000

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.

174. Ion Beam Analysis and Ion Implantation
C. W. White, M. J. Aziz, J. H. Barrett, M. K. Elghor, R. Feenstra, S. Gorbatkin, J. D. Gresset, O. W. Holland, J. C. McCallu, C. J. McHargue, D. B. Poker, O. E. Schow, J. M. Williams, S. P. Withrow
(615) 574-6295/(FTS) 624-6295 **02-5**
$1,220,000

Studies of ion implantation damage and annealing in a variety of crystalline materials (semiconductors, metals, superconductors, insulators, etc.), formation of unique morphologies such as buried amorphous or insulating layers by high dose ion implantation, the use of high-energy ion beams to reduce the temperature of various thermally activated processes such as damage removal, alloying, and phase transformations, characterization of superconducting thin films deposited by electron beam evaporation and laser ablation, 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, and to reduction of corrosive wear of surgical alloys, and to investigate application of pulsed-laser-induced localized melting for damage removal and alloy formation in ion-implanted crystals, high speed crystal growth phenomena, such as solute trapping and segregation, formation of epitaxial thin films by direct ion beam deposition, studies of ion channeling phenomena.

175. Investigations of Superconductors with High Critical Temperatures
F. W. Young, Jr., L. A. Boatner, J. Brynstead, D. K. Christen, D. M. Kroeger, S. H. Liu, H. A. Mook, B. C. Sales, S. T. Sekula, J. R. Thompson
(615) 574-5501/(FTS) 624-5501 **02-5**
$500,000

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

176. Surface Physics and Catalysis
D. M. Zehner, A. F. Baddorf, H. L. Davis, G. R. Gruzalski, J. R. Noonan, G. W. Ownby, J. F. Wendelken
(615) 574-6291/(FTS) 624-6291 **02-5**
$995,000

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 interplanar spacings different from those of the bulk, LEED, PES, and Auger electron spectroscopy (AES) combined with in situ laser irradiation of semiconductors, lineshape analysis of Auger spectra, LEED, AES and X-ray photoelectron 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 surfaces and adsorbates examined by high-resolution electron energy loss spectroscopy (EELS), examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

177. Ion Beam Deposition
R. A. Zuhr, T. E. Haynes, J. B. Roberto
(615) 576-6722/(FTS) 626-6722 **02-5**
$410,000

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, formation of compound semiconductor and metallic layers, production of oxides and thin magnetic films, and investigation of low-energy ion-solid interactions including ion beam etching and damage processes.

Materials Chemistry - 03

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

178. 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
(FTS) 624-5024/(FTS) 624-5024 **03-1**
$1,209,000

Application of ion implantation and ion beam mixing to the generation and systematic study of surface-modified materials of interest as catalysts, e.g., $M_xTi_{1-x}O_2/Ti$(M = Ru, Ir, Rh, etc.) for electrocatalysis of Cl_2 and O_2 evolution; determination of the mechanism, the specific activites, and the electronic properties of the catalysts via electrochemical, Rutherford backscattering, and in situ photoacoustic and photocurrent spectroscopic techniques. Development of new generalized methodologies for the synthesis of non-oxidic ceramic materials (BN, Si_3N_4, SiC, C-B-N ternaries, and 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; synthesis of semiconducting C-N-B thin films via pyrolysis of borazine derivatives. Synthesis of TiN whiskers via reactions of titanates with NaCN or NH_3 at high temperatures; topochemically specific solid-state reactions. Synthesis and characterization of superconducting oxides; composition/grain boundary/property relationships.

179. Nucleation, Growth, and Transport Phenomena in Homogeneous Precipitation
C. H. Byers, O. A. Basaran, M. T. Harris
(615) 574-4653/(FTS) 624-4653 **03-2**
$307,000

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).

180. Thermodynamics and Kinetics of Energy-Related Materials
T. B. Lindemer, T. G. Godsey, F. A. Washburn
(615) 574-6850/(FTS) 624-6850 **03-2**
$324,000

The objective here is the determination and chemical thermodynamic modeling of nonstoichiometry, phase equilibria, and other thermochemical data for energy-related ceramic systems. Our new adaptation of solid-solution thermodynamics is used to represent the chemical thermodynamic interrelationship of temperature, oxygen partial pressure, and nonstoichiometry in oxide compounds having extensively variable oxygen-to-metal ratios. Presently, these interrelationships are being measured and modeled for superconducting oxides in the the (Y, lanthanide)-barium-copper-oxygen systems. These efforts are providing a heretofore unavailable description of these oxides. The effects of solid-solution carbonate on superconductivity are also being studied.

181. 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
(615) 574-4974/(FTS) 624-4974 **03-2**
$1,218,000

Characterization of polymers and composites at the molecular level by neutron and X-ray scattering studies and by thermal analysis; structural relationships between crystalline, partially ordered, and amorphous regions; prediction of conformational, thermodynamic, and dynamic properties through advanced molecular dynamics simulations and statistical mechanical techniques; relationship of structure to physical properties; development of neutron spectroscopic techniques. Materials studied include high-performance crystalline fibers and composites, conducting polymers and small-molecule models for polymers.

Advanced Neutron Source - 04-1

182. Advanced Neutron Source
C. D. West, R. M. Harrington, J. B. Hayter, B. H. Montgomery, D. L. Selby, P. B. Thompson
(615) 574-0370/(FTS) 624-0370 **04-1**
$8,200,000

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. U3Si2 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.

Pacific Northwest Laboratory

P. O. Box 999
Richland, WA 99352
G. L. McVay - (509) 375-3762

Metallurgy and Ceramics - 01

G. L. McVay - (509) 375-3762

183. Microstructural Modification in Ceramic Processing Using Inorganic Polymer Dispersants
G. J. Exarhos, I. A. Aksay (U. of Wash), B. J. Tarasevich (PNL)
(509) 375-2440 **01-1**
$350,000

The goal of this program is to develop a fundamental understanding of structure-property relationships for inorganic polymer dispersants used in colloidal processing of ceramic powders. Near-term goals rely on molecular spectroscopic studies to investigate localized particle-polymer-solvent interactions. Results from these studies, integrated with particle densification measurements, suggest chemical modifications to the polymer designed to perturb these interactions and improve packing efficiency. Thermally-induced alterations of bound inorganic polymers in the greenbody during sintering are also being investigated. Improvement in mechanical properties of the fired ceramic is correlated with void densities and distributions that evolve during processing.

184. Fundamental Studies of Stress Corrosion and Corrosion Fatigue Mechanisms
R. H. Jones, D. R. Baer, M. A. Friesel, C. H. Henager, C. F. Windisch
(509) 376-4276 **01-2**
$435,000

Investigations of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium nickel, nickel-based alloys, and ceramic matrix composites in gaseous and aqueous environments. Relationships between interfacial and 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.

185. Chemistry and Physics of Ceramic Surfaces
L. R. Pederson, K. F. Ferris
(509) 375-2731 **01-3**
$359,000

Development of structure/property relationships for ceramic materials in a reactive environment is the focus of this program, using systematic variations of bulk, surface, and environmental properties. A fundamental understanding of the physics and chemistry at ceramic surfaces is evolved through correlations between experimental measurement and molecular modeling methods. Primary experimental molecular spectroscopy tools (FTIR, Raman, XPS, and MAS-NMR) are used to investigate initial structures and their evolution in chemically reacting environments. Model systems, electronic structure, and molecular dynamics approaches are emphasized in interpreting molecular-level phenomena. The combination of these techniques is used to extend the molecular information to bulk phenomena.

186. Irradiation-Assisted Stress Corrosion Cracking
S. M. Bruemmer, R. H. Jones, E. P. Simonen
(509) 376-4276 **01-4**
$200,000

The mechanisms controlling irradiation-assisted stress corrosion cracking are being evaluated through a combination of experiment and modeling. Research includes examination of radiation effects on grain boundary chemistry, crack-tip phenomena, and water chemistry. Grain boundary chemistry is being measured as a function of material and irradiation parameters. Specific grain boundary chemistries are simulated by thermal treatments and their influence on corrosion and stress corrosion assessed by tests in low- and high-temperature aqueous environments. Crack-tip chemistry models are being evolved so that radiation effects on local material microstructure/microchemistry and on water chemistry can be assessed in relation to crack propagation mechanisms.

Solid State Physics - 02
G. L. McVay - (509) 375-3762

187. Thin Film Optical Materials
G. J. Exarhos, C. B. Duke, K. F. Ferris
(509) 375-2440 **02-2**
$238,000

Theoretical and experimental investigations of basic materials properties that control the linear and non-linear optical behavior of thin film dielectrics. Extension of composite media approaches to model the complex dielectric constant of wide band-gap materials relies on experimental measurements of film molecular structure and microstructure. Phase composition, stoichiometry, strain heterogeneity, and void microstructure of deposited films, which are determined using laser spectroscopic methods and electron microscopy, are integrated into these models. Ellipsometry and optical transmission/reflection measurements on supported films are used to determine complex refractive indices; non-linear response is investigated using harmonic mixing methods. Materials studied include oxides, nitrides and uv-transparent polymers.

Materials Chemistry - 03
G. L. McVay - (509) 375-3762

188. Ceramic Composite Synthesis Utilizing Biological Processes
P. C. Rieke, I. A. Aksay, A. H. Heuer, B. J. Tarasevich
(509) 375-2833 **03-1**
$500,000

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. 0. Box 5800
Albuquerque, NM 87185
F. L. Vook - (505) 844-9304/(FTS) 844-9304

Metallurgy and Ceramics - 01
F. L. Vook - (505) 844-9304/(FTS) 844-9304

189. Physics and Chemistry of Ceramics
R. A. Assink, C. J. Brinker, B. C. Bunker, B. D. Kay, K. D. Keefer, J. A. Martin, C.H.F. Pedan, D. W. Schaefer, J. A. Voigt
(505) 846-2537/(FTS) 846-2537 **01-2**
$1,225,000

Multidisciplinary studies to relate molecular structure of ceramics to physical properties. One objective is to develop a fundamental understanding of the precursor preparation and consolidation processes required to produce novel and superior ceramics. A second objective is to study the surface chemistry of ceramics as it is relevant to consolidation. A third objective is to study interfacial reactions of ceramics as it relates to bonding and adhesion. 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. Study phase relationships in ceramic superconductors.

190. Ion Implantation and Defects in Materials
S. T. Picraux, R. J. Bourcier, K. L. Brower, B. L. Doyle, D. M. Follstaedt, J. A. Knapp, S. M. Myers, P. S. Peercy, L. E. Pope, A. D. Romig, N. R. Sorensen, H. J. Stein, W. R. Wampler
(505) 844-7681/(FTS) 844-7681 **01-3**
$953,000

Ion implantation and ion beam mixing are used with laser and electron-beam heating to form novel metastable and equilibrium microstructures in solids. The evolution and final states of these systems are characterized 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 materials, and mechanical and chemical effects of ion implantation. Investigation of consequences for semiconductor-device development, fusion energy, hydrogen storage, coatings technology and corrosion.

191. Advanced Growth Techniques for Improved Semiconductor Structures
S. T. Picraux, E. Chason, B. W. Dodson, B. L. Doyle, I. J. Fritz, K. Horn, A. W. Johnson, K. P. Killeen, J. Y. Tsao
(505) 844-7681/(FTS) 844-7681 **01-3**
$355,000

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) and atomic layer epitaxy (ALE) are used in conjunction with laser and ion beam stimulation to develop new crystal growth and diagnostic techniques. Studies concentrate on layered III-V compounds and Ge, Si, and SiGe strained layer structures, with emphasis on beam techniques to allow a wider range of nonequilibrium growth conditions and thus to widen the window of compositions and combinations of high quality materials that can be grown. Advanced in situ techniques yield surface-structure and composition information for correlation with growth parameters. Theoretical studies using atomistic and continuum modeling address growth mechanisms and beam-enhanced growth in conjunction with the above experimental studies.

192. Strained-Layer Superlattice Materials Science
P. L. Gourley, R. M. Biefeld, L. R. Dawson, B. W. Dodson, I. J. Fritz, E. D. Jones, S. K. Lyo, G. C. Osbourn, J. Y. Tsao
(505) 844-4309/(FTS) 844-4309 **01-5**
$420,000

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.

Solid State Physics - 02
G. A. Samara - (505) 844-6653/(FTS) 844-6653

193. Physics and Chemistry of Novel Superconductors
D. S. Ginley, R. J. Baughman, D. R. Jennison, J. F. Kwak, B. Morosin, J. E. Schirber, E. B. Stechel, E. L. Venturini
(505) 844-6653/(FTS) 844-6653 **02-2**
$538,000

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.

194. Tailored Surfaces for Materials Applications
T. A. Michalske, P. J. Feibelman, J. E. Houston, G. L. Kellogg, J. W. Rogers, Jr., N. D. Shinn
(505) 844-5829/(FTS) 844-5829 02-2
$633,000

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.

195. Very High Temperature Semiconducting Borides
D. Emin, T. L. Aselage, B. Morosin, C. H. Seager, A. C. Switendick, D. R. Tallant, E. L. Venturini
(505) 844-6653/(FTS) 844-6653 02-5
$516,000

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 - (505) 844-3871/(FTS) 844-3871

196. Chemical Vapor Deposition and Surface Photokinetic Research
A. W. Johnson, C. I. H. Ashby, W. G. Breiland, M. E. Coltrin, J. R. Creighton, P. Ho
(505) 844-8782/(FTS) 844-8782 03-3
$457,000

Studies of important vapor-phase and surface reactions 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. Development of predictive numerical models, which include chemical kinetics 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 and surface reactions of these laser processing techniques and application of surface measurement techniques to study the product materials.

Sandia National Laboratories-Livermore
P.O. Box 969
Livermore, CA 94551-0969
P. L. Mattern - (415) 294-2520/(FTS) 234-2520

197. Formation and Analysis of High Temperature Interfaces and Thin Films
M. Lapp, J. C. Hamilton, K. F. McCarty
(415) 294-2435/(FTS) 234-2070 01-1
$184,000

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 high-temperature ceramic superconductors, and to characterize the evolution of interfaces 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.

198. Gases in Metals/Computational Materials/Visiting Scientist Program
M. I. Baskes, M. S. Daw, T. E. Felter, S. M. Foiles, D. D. Johnson, T. Lowe, M. Mills, R. B. Phillips, S. Robinson, C. M. Rohlfing, G. J. Thomas, W. G. Wolfer
(415) 294-3226/(FTS) 234-3226 **01-2**
$1,136,000

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.

Solid State Physics - 02
W. Bauer - (415) 294-2994/(FTS) 234-2994

199. In Situ Diagnostics for Interfaces and Thin Films
M. Lapp, R. J. Anderson, J. C. Hamilton
(415) 294-2435/(FTS) 234-2435 **02-2**
$230,000

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. Recent results include real-time studies of species and reactions at interfaces, with current efforts on hydrogen and carbon monoxide adsorption, surface segregation, and carbon formation on metal crystals. Femtosecond laser techniques are used for ultrafast real-time investigations of electronic and reactive properties of bulk electronic materials and thin films.

Solar Energy Research Institute
1617 Cole Boulevard
Golden, CO 80401
R. A. Stokes - (303) 231-7625/(FTS) 327-1172

200. Semiconductor Theory
A. Zunger
(303) 231-1172/(FTS) 327-1172 **02-3**
$330,000

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/DeTe 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., $CdIn_2Se_4$), epitaxial 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 program, applied to binary and pseudobinary phase diagrams.

Stanford Synchrotron Radiation Laboratory

Stanford University
Stanford, CA 94305
A. I. Bienenstock - (415) 926-3153/(FTS) 462-3153

201. Research and Development of Synchrotron Radiation Facilities
A. I. Bienenstock, H. Winick
(415) 926-3153/(FTS) 462-3153 **04-1**
$5,906,000

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 turn-over in the Grant Research program, and some of the projects will not be continued beyond the current period.

Arizona State University
Tempe, AZ 85287

202. Mobile Ions in Fast Ion Conducting Systems
C. A. Angell, Department of Chemistry
(602) 965-7217 **01-1**
$80,500

Investigate novel materials that exhibit fast ion transport and high rates of energy dissipation on impact. Anionic conductivities in leadhalide-rich inorganic glasses, mixed anion-cation conducting glasses, mixed ionic-electronic conductivity in Na tellurovanadate glasses with high Na^+ transport, and new organic cation-containing plastic crystal conductors. Develop understanding of transport processes in these systems, explore possibility that fast processes occurring in glasses and ceramics can provide fast energy dissipation mechanism on impact, and utilize computer simulation calculations to study fast processes by dynamic graphics methods.

203. High Resolution Energy Loss Research: Si Compound Ceramics and Composites
R. W. Carpenter, Center for Solid State Science
(602) 965-4544
S. H. Lin, Department of Chemistry
(602) 965-3715 **01-1**
$125,000

High spatial resolution analytical electron microscopy investigation with a field emission source of the elemental composition and local electronic structure of small amorphous and crystalline regions in silicon carbide and silicon nitride 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.

204. Surface Structures And Reactions of Ceramics and Metals
J. M. Cowley, Department of Physics
(602) 965-6459 **02-2**
$105,000

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; scanning reflection electron microscopy, reflection electron energy loss spectroscopy, microdiffraction from sub-nanometer size regions, resonance channeling along surfaces and interfaces, nanometer-resolution imaging with secondary electrons, with or without energy filtering, and high resolution Auger analysis. Topics to be investigated include the structure of surfaces of ceramics and metals on an atomic scale, the existence of surface reconstructions, ordering and modifications induced by surface steps, observed as a function of temperature: the epitaxial relationships and chemical reactions of metals on ceramics and their dependence on surface structure, temperature and ionizing radiation: the influence of absorbed surface layers of water, oxygen or other gas on surface reactions. Specimens will include small metal particles on oxide supports, thin metal film grown on oxide surfaces and interfaces between metals and oxides or other materials viewed edge on.

University of Arizona
Tucson, AZ 85721

205. Grain Boundary Phase Equilibrium in Metallic Systems
P. A. Deymier, Department of Materials Science & Engineering
(602) 621-6080 **01-1**
$137,003

Study of properties of grain boundaries in pure metallic and alloy systems. Experiments coupled with dynamical atomistic computer simulations. Measurement and calculations 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.

206. Artificially Structured Superconductors
C. M. Falco, Department of Physics
(602) 621-6771 **02-2**
$101,349

Investigation of the nature of artificial metallic multilayer systems and ceramic superconducting thin films, their electronic and superconducting properties including their weak link characteristics. Production of superlattices and thin films with greater perfection than heretofore, and understanding of the important preparation parameters. Fabrication of materials both with a three-gun magnetron sputtering system, and by molecular beam epitaxy. Use of X-ray diffraction, resistance, Rutherford backscattering (RBS), TEM, Mossbauer spectroscopy, and electron tunneling to characterize samples. Emphasis is on the superconducting properties to develop weak links and microbridges with increased range of operating conditions.

Atlanta University

Atlanta, GA 30314-4381

207. Ceramic Mateials from Preceramic Organometallic Copolymers
Y. H. Mariam, Dept. of Chemistry
(404) 653-8593 **01-3**
$62,632

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 paths. Correlation of chemical intermediate characteristics with ceramic, microstructural, microchemical, and micromechanical properties.

Boeing Aerospace Company

Seattle, WA 98124

208. X-ray Spectroscopic Investigation of Radiation Damaged Materials
R. B. Greegor, Physics Technology
(206) 544-5307
F. W. Lytle, P. O. Box 3999
(206) 655-5574 **01-1**
$70,170

Extended X-Ray Absorption Fine Structure (EXAFS/XANES) techniques are used to determine the structural arrangements in natural minerals that are found to various extents in the metamict state. These minerals include titanates, zircons, thorites, monazites, huttonites, furgusonites, and perovskites. Comparisons are made with synthetic minerals doped with actinides (Pu) and self-damaged, damaged by ion-irradiation, or otherwise radiation damaged.

Boston University

590 Commonwealth Avenue
Boston, MA 02215

209. Studies of Transition Metal Surfaces and Overlayers Dynamics and Magnetism by He and Spin Polarized Metastable He Beam Spectroscopies
M. M. El-Batanouny, Department of Physics
(617) 353-4721 **02-4**
$107,000

Use of scattered spin-polarized metastable $He(2^3S)$ atoms from surfaces both elastically and inelastically, to study the structural, dynamic and magnetic trends of the 3D transition metal overlayers-Cr and Fe on Pd(110), Pd(111) and CU(100) substrates. Magnetic properties will be studied in the newly constructed Spin-Polarized Metastable He (SMPH) facility. Computer modeling, employing Friedel oscillations and Double-sine-Gordon surface dislocations, will be used to interpret the Au(111) measured phonon dispersion data.

Brandeis University

Waltham, MA 02254

210. Synthesis and Properties of Novel, Electroactive Organometallic Polymers
M. Rosenblum, Department of Chemistry
(617) 647-2807 **03-1**
$16,464 (11 months)

Synthesis of organometallic polymers based on transition metal complexion 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.

Brown University
Providence, RI 02912

211. Fatigue Crack Growth Under Far-field Cyclic Compression
S. Suresh, Division of Engineering
(401) 863-2626 **01-2**
$94,731

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 temperature from which guidelines for fatigue design involving advanced engineering materials will evolve.

212. Surfaces and Thin Films Studied by Picosecond Ultrasonics
H. J. Maris, Department of Physics
(401) 863-2185
J. Tauc, Division of Engineering and Department of Physics
(401) 863-2318 **02-2**
$154,600

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 durations 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 non-destructive testing technique of 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

213. Ordering Phenomena In Undercooled Alloys
B. T. Fultz, Engineering Department
(818) 356-2170 **01-1**
$84,999

This research is intended to address fundamental questions concerning the motion and interaction of atoms in metallic alloys. A study of vibrational entropy contribution to the thermodynamics of the order-disorder transformation. Mossbauer spectrometry will be used to study the evolution of local atomic arrangements in undercooled Fe_3Al. 3d and 4d charge transfers will be related to enthalpies of phase transformations. Monte Carlo simulations of short range ordering by vacancy diffusion will address kinetic issues, such as vacancy trapping.

214. Studies of Alloy Structures and Properties
W. L. Johnson, Division of Engineering and Applied Science
(818) 356-4433 **01-1**
$232,995

Study of stability of crystalline metallic solids far from equilibrium and t their tendency to undergo crystalline to glass transformations. Development of an understanding of how severe mechanical deformation of powders of pure metals and intermetallic compounds alters the materials properties. Research on hydrogen-induced phase transformations, especially amorphization in rare earth/transition metal Laves phases. Study of the properties of thin films of metallic solid solution phases at non-equilibrium concentrations. Examination of evolution of chemical disorder in intermetallic compounds under ion irradiation and characterization of physical properties. Study of pressure as a means of inducing the crystalline to glass transformation. Phenomenological modeling and computer simulation. Examination techniques include X-ray and electron diffraction, specific heat, thermal expansion coefficient, and Mossbauer spectroscopy.

215. Grain Boundary and Interface Kinetics During Ion Irradiation
H. A. Atwater, Department of Applied Physics
(818) 356-2197 **01-4**
$92,696

Experimental study of interface motion and stability in polycrystalline thin films during ion irradiation. Relation of the structure and density of collision cascades produced during irradiation to the kinetics of grain boundary motion. Microstructures compared with binary collision-based Monte-Carlo simulations of cascade structure, phenomenological models of thermal spike formation, and data from molecular dynamics simulation of high density cascades. Results used to test analytic theories of cascade evolution. Relation of grain boundary and interface structure to their stability with respect to the crystal-to-amorphous transition under irradiation. In situ electron microscopy and optical interferrometry used to determine interface structures, velocities and morphology. Post-irradiation electron microscopy and grain size measurements used to examine interface structure and evolution of film microstructure. Results compared with models of grain boundary structure and grain boundary melting.

216. Melting In Adsorbed Films
D. L. Goodstein, Department of Physics, Mathematics, and Astronomy
(818) 356-4319 02-2
$106,000

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.

University of California at Davis
Davis, CA 95616

217. 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
(916) 752-1863
A. K. Mukherjee, Dept. of Mechanical Engineering
(916) 752-1776 01-2
$130,094

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.

218. Radiation Damage and Decomposition of Ceramics by Electron Microscopy
D. G. Howitt, Department of Mechanical Engineering
(916) 752-0580 01-4
$120,000

Investigation of electron and ion irradiation induced ionization, displacement damage, diffusion, and stimulated desorption by means of in-situ analytical electron microscopy and mass spectroscopy. Study of ion mixing effects under ion irradiation. Materials include dielectrics and semiconductors. Study of free standing ceramics thin films.

219. An Investigation of the Mechanisms of Self-propagating High Temperature Synthesis Reactions
Z. A. Munir, Dept. of Mechanical Engineering
(916) 752-0559 01-5
$68,000

Investigation of the mechanisms of reactions associated with self-sustaining combustion synthesis. Characterization of combustion wave velocities and temperature profiles. Determination of activation energies. Effects of powder size and distribution, surface layers, thermal history, gas pressure, and ignition temperature. Materials investigated include transition metal carbides and nitrides and laminated thin metallic foils in the Ni-Al system.

University of California at Irvine
Irvine, CA 92717

220. Optical Studies of Molecular Adsorbates
J. C. Hemminger, Department of Chemistry
(714) 856-6020 02-2
$159,120

Investigation, by means of Raman scattering spectroscopy, of 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 and laser induced thermal desorption.

221. Inelastic Electron Scattering from Surfaces
D. L. Mills, Department of Physics
(714) 856-5148 **02-3**
$127,638 (10 months)

Theory of the inelastic scattering of electron, 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-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 Mills and Professor Tong at the University of Wisconsin at Milwaukee.

University of California at Los Angeles
Los Angeles, CA 90024

222. Irradiation-Induced Disordering, Ductility and Phase Transformations in Ordered Intermetallic Compounds
A. J. Ardell, Department of Materials Science and Engineering
(213) 825-7011 **01-4**
$85,800

Proton irradiation of ordered intermetallic compounds at temperatures from -175°C to room temperature. Investigation of irradiation-induced ductility in $L1_2$ and B2 compounds. Irradiated specimens mechanically tested in bending, and fracture surfaces studied for assessment of ductility. Specimen examination by TEM, X-ray diffraction, and electron diffraction. Identification and characterization of tweed-like reaction product of a phase transformation in proton-irradiated hypostoichiometric Ni_3Al.

223. Quantum Fluctuations in Mesoscopic Systems
SheChao Feng, Department of Physics
(213) 825-8530 **02-3**
$60,000

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.

224. Experimental Studies of Solitons, Fractons, and Wave Turbulence in Continuous Media
G. A. Williams, Department of Physics
(213) 825-8536
S. Putterman, Physics Department
(213) 825-8536 **02-5**
$125,000 (16 months)

Investigation of the nonlinear dynamics in continuous media will be performed. Novel soliton structures will be examined, including standing-wave kink solitons. Envelope solitons in a cylindrical metallic shell will be investigated further. Studies on the nucleation of the A–B transition of ^3He will be completed.

University of California at San Diego
La Jolla, CA 92093

225. Superconductivity and Magnetism in D- and F- Electron Materials
M. B. Maple, Department of Physics
(619) 534-3330 **02-2**
$350,000

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 (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 kilobar. Search for new high T_c superconducting materials and characterization of their properties, including 4f electron hybridization effects, magnetic ordering, growth of single crystals and measurement of upper critical fields and critical current densities.

226. Preparation and Characterization of Superlattices
I. K. Schuller, Department of Physics
(619) 534-2540 02-2
$104,000

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.

227. Ion Mixing and Surface Modification in Metal Semiconductor Systems
S. S. Lau, Department of Electrical Engineering and Computer Sciences
(619) 534-3097
J. Mayer, Cornell University, Department of Materials Sciences and Engineering, Ithaca, NY 14853
(607) 255-7273 02-4
$135,000

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 at Santa Barbara

Santa Barbara, CA 93106

228. Structure and Chemistry of Metal/Ceramic Interfaces
M. Ruhle, Materials Department
(805) 961-8275 01-1
$110,000

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.

229. Condensed Matter Research Using the USCB Free Electron Laser
V. Jaccarino, Department of Physics
(805) 961-2121 02-2
$73,000

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.

230. Research in Theories of Pattern Formation and Nonequilibrium Processes
J. S. Langer, Department of Physics
(805) 961-3247 02-3
$130,000

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.

231. Numerical Simulation of Quantum Many-Body Systems
D. J. Scalapino, Department of Physics
(805) 961-2871
J. R. Schrieffer, Physics Dept.
(805) 961-2800
R. L. Sugar, Physics Dept.
(805) 961-3469 02-3
$120,000

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, 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.

232. Molecular Properties of Thin Organic Interfacial Films
J. Israelachvili, Department of Chemical and Nuclear Engineering
(805) 961-2902 **03-1**
$170,000

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.

233. Polymers at Surfaces
P. A. Pincus, College of Engineering-Engineering Materials Program
(805) 961-4362 **03-2**
$100,000

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 adsorbed on fluid-fluid interfaces. Dispersion stability of suspended colloids with adsorbed 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 at Santa Cruz
Santa Cruz, CA 95064

234. Experimental Studies of Critical Behavior in Systems With Quenched Disorder
D. Belanger, Department of Physics
(408) 429-2871 **02-1**
$80,999

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.

Carnegie Mellon University
3325 Science Hall
Pittsburgh, PA 15213

235. The Effects of Applied Stress on Microstructural Evolution
W. C. Johnson, Department of Metallurgical Engineering and Materials Science
(412) 268-8785 **01-1**
$74,932

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.

236. Phase Separation and Ordering in InGaAsP and InGaAs Materials
S. Mahajan, Department of Metallurgical Engineering and Materials Sciences
(412) 268-2702
D. E. Laughlin, Department of Metallurgical Engineering and Materials Sciences
(412) 268-2706 **01-1**
$165,000

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.

237. Equilibrium Composition of Interphase Boundaries
P. Wynblatt, Department of Metallurgical Engineering and Materials Science
(412) 268-8711 **01-1**
$105,000

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.

238. Theoretical Models for the Ultimate Strength and Flaw Resistance of Undirectionally-Reinforced Ceramic-Matrix Composites
P. S. Steif, Department of Mechanical Engineering
(412) 268-3507 **01-2**
$100,000

Theoretical study of the microstructural determinants of strength and toughness in fiber-reinforced ceramics. Macroscopic properties include: the ultimate tensile strength parallel to the fibers and the resistance to matrix flaws which propagate normal to the fiber direction. Understand the extent to which these macroscopic properties depend on critical micro-level properties, including, the character of the fiber-matrix interface, as well as the fiber and matrix moduli, strength and strength variability. Theoretical approach to incorporate the influence of the interface via micromechanics models of the interface, that reflect either the presence of chemical bonding or the possibility of interfacial slippage.

University of Chicago
5640 Ellis Avenue
Chicago, IL 60637

239. High-Temperature Thermochemistry of Transition Metal Borides and Silicides
O. J. Kleppa, The James Franck Institute
(312) 702-7198 **01-3**
$60,000

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 stems.

240. Research in Two Dimensional Critical Phenomena and Conformal Field Theory
D. Friedan, Enrico Fermi Insitute
(312) 702-7119
S. Shenker, Enrico Fermi Institute
(312) 702-7187 **02-3**
$100,000

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 tricritical 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 45221-0172

241. Surface Chemistry of Electrocatalysts
A. Hubbard, Department of Chemistry
(513) 475-2263 **03-2**
$60,000

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 sulfoixde, promoters such as iodide, and poisons such as carbon monoxide and aminoethanethiol on surfaces of copper, silver, gold, platinum, and alloys of these elements.

Clark College
Atlanta, GA 30314

242. Investigation of Polling Processes, Charge Trapping and Preservation in Some Ferroelectric and Polymeric Materials
O. P. Puri, Division of Natural Sciences and Mathematics
(404) 681-8161, ext. 200 **01-3**
$80,900

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 analyses on oxides, chalcogenide, and elemental Si samples.

Colorado School of Mines
Golden, CO 80401

243. The Role of Composition and Microstructure Gradients on Weld Metal Properties and Behavior
D. L. Olson, Center for Welding and Joining Research
(303) 273-3787
D. K. Matlock, Center for Welding and Joining Research
(303) 273-3775 **01-5**
$130,000

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.

244. Physical and Electronic Structure of the Electrolyte-Solid Interface Through Optical Phenomena
T. Furtak, Department of Physics
(303) 273-3843 **02-2**
$65,000 (6 months)

Development and application of techniques for the investigation of electrochemical environments, specifically solid-electrolyte interfaces. In situ optical experiments including Raman and second harmonic generation spectroscopy and scanning tunneling microscopy will be employed. Investigation of the interrelationships between substrate crystallography and microstructure and the electrochemical parameters subject to external control will be performed. Emphasis is on model systems such as silver and platinum with well-defined amounts of foreign metal atoms and/or inorganic ions in contact with the surface.

Colorado State University
Fort Collins, CO 80523

245. Properties of Molecular Solids and Fluids at High Pressure and Temperature
R. D. Etters, Department of Physics
(303) 491-5374 02-3
$74,550

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 viral 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, I_2, Cl_2, Br_2, HI, HBr, and H_2. Attention is given to connections with combustion and detonation phenomena, and to synthesis of new materials. Collaboration with theoretical work and close correlation with experimental programs at LANL and LLNL continues.

University of Colorado
Boulder, CO 80309

246. Dynamic and Static Features of the 2d Melting/Freezing Process
W. J. O'Sullivan, Department of Physics
(303) 492-7547
R. C. Mockler, Dept. of Physics
(303) 492-8511 02-2
$50,000

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

247. Protons and Lattice Defects in Perovskite-Related Oxides
A. S. Nowick, Krumb School of Mines
(212) 854-2921 01-3
$128,000

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 divalent or trivalent transition-metal ions. Carrier analysis by thermoelectric power measurements. Electrical conductivity measurements as a function of temperature and controlled environment. Impedance measurements and analysis to determine lattice and grain boundary conductivity. IR measurements to determine proton content. Behavior and defect chemistry of hydrogen containing samples. Characterization of the effect of equilibration of superconducting oxides with known partial pressures of oxygen and hydrogen.

University of Connecticut
Storrs, CT 06268

248. A Coherent Model of Martensitic Nucleation and Growth
P. C. Clapp, Department of Metallurgy
(203) 486-4714 01-1
$125,396

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. Comparisons to experimental data on Na, β-NiAl, Fe-3ONi and Nb_3Sn.

249. Fatigue of Ferritic and Austenitic Steels at Elevated Temperatures
A. J. McEvily, Department of Metallurgy
(203) 486-2941 **01-2**
$37,761

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.

Cornell University
Ithaca, NY 14853

250. Crystalline-Amorphous Oxide Interfaces and Their Relation to Grain Boundary Films
C. B. Carter, Department of Materials Science and Engineering
(607) 255-4797 **01-1**
$160,000

Study of the structure and chemistry of the interface between an amorphous material and a crystalline one. Surface reaction on a bicrystal sample examined by cross-sectional transmission electron microscopy and reaction of a glass-forming vapor with a pre-thinned TEM sample. Materials studied are alumina, magnesia and silicon.

251. Strong Fibers
H. H. Johnson, Department of Materials Science and Engineering
(607) 255-2323 **01-1**
$130,000

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.

252. Focal Problems in Modulated and Martensitic Structural PhaseTransformations in Alloys and Perovskites
J. A. Krumhansl, Dept. of Physics
(607) 255-5261 **01-1**
$135,000

New theoretical approach to a microscopic description of martensitic transformations of the twinning type, based on nonlinear, nonlocal elastic displacement fields. Results applicable to both alloy martensitic transformations and high-T_c 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 psuedo-critical behavior, and anomalous behavior in structural transitions.

253. Studies of the III-V Compounds in the Megabar Regime
A. L. Ruoff, Department of Materials Science and Engineering
(607) 255-4161 **01-1**
$131,000

Crystal structure changes in the III-V compounds as a function of pressure to 200-300 GPa (2-3 Mbar) with emphasis on the transformation from four-fold to sixfold 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.

254. Experimental and Theoretical Studies of the Structure of Grain Boundaries
S. L. Sass, Deparment of Materials Science and Engineering
(607) 255-5239 **01-1**
$165,900

Investigation of grain boundary structure of BCC metals, ceramics, and intermetallic compounds using transmission electron microscopy, 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, determination of grain boundary region in order to obtain structural information.

255. UHV-Stem Studies of Nucleation and Growth of Thin Metal and Silicide Films on Silicon
J. Silcox, School of Applied and Engineering Physics
(607) 255-3332
E. J. Kirkland, School of Applied and Engineering Physics
(607) 255-3332 **01-1**
$131,000

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.

256. Interface Science in Deformation Processing of Ceramics
Rishi Raj, Department of Materials Science & Engineering
(607) 255-4040 **01-2**
$224,953 (10 months)

Investigate 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 grain boundaries over appropriate stoichiometric and applied stress intervals. Theoretical modeling of chemical diffusion and deformation processes using acquired experimental data.

257. Structure and Electronic Properties of Mismatched III-V Interfaces
D. Ast, Department of Materials Science and Engineering
(607) 255-4140 **01-3**
$94,000

Study the structure, electrical properties, stability and suppression of interface defects in lattice mismatched III-V systems and related systems. Investigation includes single overlayer and multiple overlay growth (superlattices) on flat substrates and patterned substrates. Develop a thorough understanding on what factors promote the formation of interface dislocations.

258. Surface Phases and Their Influence on Metal-Oxide Interfaces
J. M. Blakely, Department of Materials Sciences and Engineering
(607) 255-5149 **01-3**
$114,363

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.

259. Defects and Transport in Mixed Oxides
R. Dieckmann, Department of Materials Science and Engineering
(607) 255-4315 **01-3**
$138,150

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.

260. The Geometry of Disorder: Theoretical Investigations of Quasicrystals and Frustrated Magnets
C. I. Henley, Department of Physics
(607) 255-9684 **02-3**
$76,401

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.

261. Synthesis and Properties of Novel Cluster Phases
F. J. DiSalvo, Department of Chemistry
(607) 255-7238 **03-1**
$145,568

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

262. The Structure and Properties of Grain Boundaries in B2 Ordered Alloys
I. Baker, Thayer School of Engineering
(603) 646-2184 01-2
$95,001

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.

263. Intergranular Fracture and the Accommodation of Slip at Grain Boundaries
E. M. Schulson, Thayer School of Engineering
(603) 646-2888 01-2
$120,037

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 (0.35 at%) 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 (0.35 at%) and without boron; investigate grain size effects on the strength and ductility of Ni_3Si, Ni_3Ge, and Ni_3Ga by systematic experiments on the effects of grain size on the mechanical properties and resultant deformation structure; improve the toughness of intermetallic compounds through grain shape control, i.e., generate equiaxed fine grain structure with simultaneous increase of aspect ratio, comparative tests (fibrous vs equiaxed microstructures) performed at RT using Charpy impact technique. Subsequent fracture toughness measurements using standard ASTM procedures.

University of Delaware
Newark, DE 19716

264. Neutron Studies of Liquid and Solid Helium
H. R. Glyde, Department of Physics
(302) 451-2661 **02-1**
$65,000

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 ^3He for comparison with existing data to test models of the effective interactions between atoms in the liquid, calculations of the momentum distribution in liquid ^3He and in solid ^4He for comparison with experiments at IPNS(ANL) and to test the impulse approximation using models appropriate to solid ^4He. Development of a microscopic theory of liquid ^3He 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

265. Residual Stresses in Fiber-Reinforced Ceramic Composites by Diffraction Methods
P. K. Predecki, Department of Engineering
(303) 871-3570 **01-2**
$60,000

Investigation of residual stresses and strains in ceramic fiber/ceramic matrix composites by X-ray diffraction to obtain the near surface stresses and by 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 has been varied. Materials investigated include alumina fibers in silicate glasses and SiC whiskers in alumina. Noyan-Cohen analysis accounting for 3-dimensional nature of stresses and including, where possible, separation of macrostresses and microstress componenets 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 employed are useful for predicting the strength, toughness, and thermal expansion of these materials.

266. Investigate Fracture Toughness and Fracture Mechanisms Using Acoustic Emission Measurements
S. H. Carpenter, Physics Department
(303) 871-2176 **01-5**
$65,000

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

267. Visualization of Convection in ^{3}He-Superfluid-^{4}He Mixtures
R. P. Behringer, Department of Physics
(919) 684-8140 **02-3**
$20,000

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 ^3He 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 Atlantic University
Boca Raton, FL 33431

268. Theoretical Studies of Metallic Alloys
J. S. Faulkner, Department of Physics
(407) 367-3429
L. T. Wille, Department of Physics
(407) 367-3429 **01-1**
$70,000

Techniques for total energy calculations developed within the framework of the KKR-CPA and the non-muffin tin quadratic KKR (QKKR) band theory method. The energies, $Ex(K_i)$, calculated from the embedded cluster method (ECM) and the energies of the ordered phases will be obtained with the QKKR. The sub-programs will be integrated using a QKKR-CPA and advanced coding for a supercomputer such as bit mapping and logical operations that will lead to a vectorized code. Realistic first principles calculations of phase diagrams and phase stability parameters will then be performed on the alloys such as PdRh, MoCr, MoNb, MoTa and other topical systems.

Florida State University
Tallahassee, FL 32306

269. He-Atom Scattering Apparatus for Studies of Crystalline Surface Dynamics
J. G. Skofronik, Department of Physics
(904) 644-5497
S. A. Safron, Dept. of Chemistry
(904) 644-5239 **02-4**
$135,000

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. Surface of active metals (Ni, Cu), both clean and with physisorbed or chemisorbed layers. Surface phonon anomalies in high T_c superconductors. 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

270. The Coupling of Thermochemistry and Phase Diagrams for Group III-V Semiconductor Systems
T. J. Anderson, Department of Chemical Engineering
(904) 392-2591 **01-3**
$85,000

Component activities measured in the compound semiconductor system Ga-In-As-P with solid-state electrochemical methods. Ga or In activities measured in liquid solutions with a galvanic cell using yttria-stabilized zirconia as the solid electrolyte. Activity of GaAs in the solid solution $Ga_xIn_{1-x}As$ measured with a galvanic cell. GaAs solidus measured by coulometric titration in an electrochemical cell using MOCVD deposited GaAs. Reference state for Group III arsenides and phosphides will be studied. Infinitely dilute solutions of As or P in In and Ga will be investigated as suitable reference states. Measurement results and reference state characterization studies used to assess the thermochemistry and phase diagram of the Ga-In-As-P system. Results of this assessment will be used for complex chemical equilibrium calculations as applied to hydride CVD in $In_xGa_{1-x}As_yP_{1-y}$. Assessment of Ga-As-Bi and Al-Ga-In-P systems will be performed.

271. X-ray Scattering Studies of Non-Equilibrium Ordering Processes
S. E. Nagler, Department of Physics
(904) 392-8842 **02-2**
$65,000

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 the role of topological defects in the growth of ordered domains in the thin film samples.

272. Studies of Heavy Fermion Systems
G. R. Stewart, Department of Physics
(904) 392-9263/0521 02-2
$92,000

Experimental investigations of "heavy fermion" systems with emphasis on UBE_{13}. Use of microcalorimetry measurement techniques, coupled with applied magnetic fields up to 15T (up to 30T at National Magnet Lab.), and specific heat determinations (0.3 to 150 K) to explore similarities between single crystals of high T_c superconductors and heavy fermion superconductors. In particular, possible connections of superconductivity and magnetic correlations, highly correlated electrons, short (~10 A) superconducting correlation lengths will be examined. Doping on the non-f-atom site in UBe_{13} with B, Ga, and Al will provide new materials for study.

Georgia Tech Research Corporation
Atlanta, GA 30332

273. Study of High Tc Superconducting Thin Films Grown by MOCVD and MO-MBE
A. Erbil, School of Physics
(404) 894-5207 02-2
$90,000

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.

274. Structure and Dynamics of Material Surfaces, Interphase-Interfaces and Finite Aggregates
U. Landman, School of Physics
(404) 894-3368 02-3
$185,000 (11 months)

Numerical simulations/molecular dynamics investigations of the fundamental processes that determine the structure, transformations, growth, electronic properties and reactivity of materials and material surfaces. Focus on (1) surfaces, interfaces and interphase-interfaces under equilibrium and nonequilibrium conditions and (2) finite material aggregates. Modeling uses molecular dynamical and quantum mechanical path-integral numerical methods.

275. Growth, Structure and Stability of Epitaxial Overlayers
A. Zangwill, Department of Physics
(404) 894-7333 02-3
$82,000

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.

276. The Organic Chemistry of Conducting Polymers
L. M. Tolbert, Department of Chemistry
(404) 894-4043 03-1
$95,000

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

277. Optical Studies of Dynamical Processes in Disordered Materials
W. M. Yen, Department of Physics and Astronomy
(404) 542-2485 02-2
$125,000

Investigation 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. Application of advanced laser techniques, including fluorescence line narrowing (FLN) and time-resolved FLN, Dilution

Narrowed Laser Spectroscopy (DNLS), measurement of coherent optical transients, photoacoustic and photocaloric methods, and far infrared free electron laser. Examination of activated materials with proven fractal dimensions and properties, energy transfer across order-disorder environment.

Harvard University
Cambridge, MA 02138

278. Measurements of Crystal Growth Kinetics at Extreme Deviations from Equilibium
M. J. Aziz, Division of Applied Science
(617) 495-9884 **01-1**
$100,000

Time-resolved measurements of optical reflectance, transient electrical resistance and thermal emf will be used to measure the location, speed and temperature of rapidly moving soiid/liquid interfaces created by short laser pulses. Post-irradiation analysis will determine the resulting phase, microstructure and composition profile. Results obtained on metals and semiconductors will be compared to theories for the kinetics of solute incorporation during rapid crystal growth, the cellular or dendritic breakdown of an initially planar interface, and the undercooling at a moving interface.

279. X-ray Standing Wave Interferometry-Optics at 1 Angstrom with Applications to Surface and Material Sciences
J. A. Golovchenko, Department of Physics
(617) 495-3905 **02-2**
$175,000

Examine thin films and epitaxial growth processes using X-ray standing wave interferometry. Develop new applications of dynamical diffraction methods for investigating condensed matter. Investigate nonperturbative and nonlinear interactions of X-rays with materials. Determine the role of single atomic layers at metal-semiconductor interfaces which serve as diffusion barriers, Schottky barrier modifiers or as VLS crystal growth barrier reducers.

280. Fundamental Properties of Spin-Polarized Quantum Systems
I. F. Silvera, Department of Physics
(617) 495-9075 **02-2**
$204,824

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 using microwave traps and cooling and by using helium walls covered with electrons. 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 system by means of "third sound" resonance. Develop a matter wave interferometer.

University of Houston
Houston, TX 77004

281. Diffraction Studies of the Properties of Glasses and Liquids
S. C. Moss, Department of Physics
(713) 749-2840 **02-1**
$232,500

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
650 Harry Road
San Jose, CA 95120-6099

282. Segmental Interpenetration at Polymer-Polymer Interfaces
T. P. Russell, Almaden Research Center
(408) 927-1080
W. W. Fleming, Almaden Research Center
(408) 927-1080 **03-2**
$104,476

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

Indiana University

Bloomington, IN 47402

283. High-Resolution Electron Energy Loss Studies of Surface Vibrations

L. Kesmodel, Department of Physics
(812) 335-0776 02-2
$98,000

Investigation of surface vibrational properties on metal and semiconductor surfaces with and without absorbed 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

284. Investigation of the Processes Controlling the Flame Generation of Refractory Materials

J. L. Katz, Dept of Chemical Engineering
(301) 338-8484 01-3
$70,000

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 studies include silica, titania, alumina and germania.

Kansas State University

Manhattan, KS 66506

285. Fundamental Studies of Strongly Magnetic Rare Earth-transition Metal Alloys

G. C. Hadjipanayis, Department of Physics
(913) 532-6786 02-2
$24,820

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 sputtering 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 histories. Work in collaboration with the University of Nebraska.

Lehigh University

Bethlehem, PA 18015

286. Analytical Electron Microscopy of Catalysts

C. E. Lyman, Department of Metallurgy and Materials Engineering
(215) 861-4249 01-1
$115,765

Elucidation of the processes or phenomena which control the internal distribution of deposited metal during the preparation of supported metal catalysts. Measurement of the distribution of noble and metallic catalytic poisons on a micrometer to nanometer scale by electron beam microanalytical methods. Correlation of catalyst microstructure with catalytic activity. Variable experimental parameters include noble metal type, impregnation procedure, drying rate, reduction rate, type of So_a sorbent coating, regeneration scheme, etc. Detailed study of effects of electron beam damage on surface mobility of catalytic poisons. Principle analytical techniques are analytical electron microscopy with a field emission gun and a lateral spatial resolution better than 2 nm and electron probe elemental microanalysis with a spatial resolution of 1 to 10 μm.

287. Analytical Electron Microscopy Studies of Interfaces and Phase Transformations in Zirconia Ceramic Systems
M. R. Notis, Department of Metallurgy and Materials Sciences
(215) 758-4225 **01-1**
$118,190

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 zirconia-based eutectics. Effects of ternary additions on the growth kinetics of precipitates in magnesia partially stabilized zirconia.

288. The Effect of Point Defects and Stoichiometry on Structural Phase Transitions
J. Toulouse, Department of Physics
(215) 758-3960 **01-1**
$60,000

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 MnF_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 $PbZr(Sc,Mg)O_3$.

289. Corrosion Fatigue of Iron-Chromium-Nickel Alloys: Fracture Mechanics and Chemistry
R. P. Wei, Department of Mechanical Engineering and Mechanics
(215) 758-3587 **01-2**
$136,900

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.

Massachusetts Institute of Technology
Cambridge, MA 02139

290. Grain Boundaries
R. W. Balluffi, Department of Materials Sciences and Engineering
(617) 253-3349
P. D. Bristowe, Department of Materials Sciences and Engineering
(617) 253-3326 **01-1**
$395,000

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 Au, Al, and Ge. Experimental techniques employed include X-ray diffraction, high-resolution and conventional electron microscopy, and computer simulation.

291. Deterministic Analysis of Processes at Corroding Metal Surfaces and the Study of Electrochemical Noise in These Systems
R. M. Latanision, Department of Materials Science and Engineering
(617) 253-4697
P. C. Searson, Department of Materials Science and Engineering
(617) 253-4697 **01-1**
$75,000

The research is composed of two parts: (a) Experimental studies of the nature of potential or current fluctuations in different corrosion systems, and correlation of the results obtained with a mathematical model describing electrode fluctuations and (b) Identification of the sites of electrochemical processes occurring on electrodes by modelling the corrosion processes on an atomistic scale. Rate of the metal dissolution reaction and of the hydrogen evolution reaction and passivation vary depending upon the given site. The contribution of different lattice sites generate fluctuations in electrode potential over small time intervals. Study several metals which do not absorb hydrogen and which exhibit simple dissolution kinetics. Test specimens mostly in the form of single crystals. Cathodic and anodic processes studied separately to analyze only one partial reaction. The metals investigated are Zn, Cu, Ag, Au, Cd, Ga, and Cr.

292. Brittle-to-Ductile Transition in Cleavage Fracture
A. S. Argon, Department of Mechanical Engineering
(617) 253-2217 **01-2**
$82,221

Investigate the rate controlling process 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 dislocation 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, WMg0, 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 $T_{B\text{-}D}$ on loading rate. The experiments of Fe-3%Si and W with constant stress intensity geometry compared with models of time dependent crack-tip shielding governed by dislocation mobility.

293. Grain Boundary Nonstoichiometry in Multicomponent Ceramics
Y-M. Chiang, Materials Science & Engineering
(617) 253-6471 **01-2**
$110,000

Investigate 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, and strontium/barium titanates. 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.

294. Superconductivity and Magnetism in Rapidly Solidified Perovskites
G. Kalonji, Department of Materials Science and Engineering
(617) 253-6863
R. C. O'Handley, Department of Materials Science and Engineering
(617) 253-6913 **01-3**
$132,000

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.

295. Structural Disorder and Transport in Ternary Oxides with Pyrochlore Structure
H. L. Tuller, Dept. of Materials Science and Engineering
(617) 253-6890 **01-3**
$100,000

Relationship of electrical and optical properties to the defect structure in ternary and quaternary oxides with the pyrochlore structure. Use of transition elements to alter electronic properties, rare-earth elements to alter the ionic conduction characteristics, and aliovalent dopants to change the carrier concentrations. Numerical calculations of the transport and structural parameters of these systems. Structural disorder characterized by X-ray diffraction, neutron diffraction, and spectroscopic measurements. Electrical characterization by AC impedance techniques. Materials to be doped and studied include the Gd_2O_3-ZrO_2-TiO_2 and Y_2O_3-ZrO_2-TiO_2 systems.

296. Mechanisms of the Oxidation of Metals and Alloys
G. J. Yurek, Department of Materials Science and Engineering
(617) 253-3239 **01-3**
$234,000

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 ratios 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 oxide scale grain boundaries will be examined.

297. Radiation Disorder and Aperiodicity in Irradiated Ceramics
L. W. Hobbs, Department of Materials Science & Engineering
(617) 253-6835 **01-4**
$115,000

Fundamental study to characterize irradiation-induced amorphization of network silicas and pyrophosphates. Irradiations to be performed in situ with electrons in a TEM or with heavy ions using the implantation facilities at ORNL. Characterization by electron diffraction, high-resolution imaging, Rutherford backscattering, optical reflectivity, and high-performance liquid chromatographic techniques. Four polymorphs of SiO_2, representing three very different combinatorial geometries in their network structures, and single crystals of $Pb_2P_2O_7$ will be studied. A topological approach will be used in computer simulations to model the amorphization.

298. Identification of Nitriding Mechanisms in High Purity Reaction Bonded Silicon Nitride
J. Haggerty, Materials Processing Center
(617) 253-2139 **01-5**
$93,487

Nitriding studies of 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 solids.

299. The Mathematical Modelling of Arc Welding Operations
J. Szekely, Department of Materials Science & Engineering
(617) 253-3236 01-5
$95,000

Development of an improved fundamental understanding of heat flow and fluid flow phenomena in arc welding operations through mathematical modelling; improvement of the ability to relate structure and properties of the weldments to operating conditions. Major thrust areas include the study of the behavior of fully three dimensional weldpools, the effects of free surface behavior, and the interactions between the welding arc and the weldpool surface. The modelling efforts interact with an experimental program at Oak Ridge National Laboratory.

Miami (Ohio) University
Oxford, OH 45056

300. Investigation of Magnetic Anisotropy and Spin Wave Modes in Transition Metal Multilayers
M. J. Pechan, Department of Physics
(513) 529-4518 02-2
$38,000

Investigation of magnetic multilayers using ferromagnetic resonance. Measurements of the magnetic interface anisotropy as a function of layer thickness, temperature, and frequency. Develop and use a variable temperature torque magnetometer to measure dc multilayer anisotropy and magnetization. Model the effects of magnetization gradients and interface frustration on interface anisotropy.

Michigan State University
East Lansing, MI 48824

301. 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
(517) 353-9767 01-2
$75,000

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

302. Effects of Gradients on Boundary Stability
S. Hackney, Metallurgical Engineering Department
(906) 487-2170 **01-1**
$100,000

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.

303. Local Chemistry and Mechanical Behavior in Stress Corrosion Cracking and Liquid Metal Embrittlement
L. A. Heldt, Department of Metallurgical Engineering
(906) 487-2630 **01-2**
$69,999

Parallel studies of stress corrosion cracking (SCC) and liquid metal embrittlement (LME), 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 LME cracks, (2) simulation of the solution chemistry within SCC cracks, (3) measurement of crack propagation velocities as influenced by chemical/electrochemical environment, stress intensity, and temperature, and (4) detailed microscopic studies of resultant fracture surfaces.

University of Michigan

Ann Arbor, MI 48109-2136

304. Micromechanical and Microstructural Studies of Ceramic Superplasticity
I-W. Chen, Department of Materials Science & Engineering
(313) 763-6661 **01-2**
$97,000

Pressure-aided superplasticity in single and poly-phase ceramics. Experiments with dense isostructural ceramics (ZrO_2-CeO_2, CaF_2-SrF_2, and $YBa_2Cu_3O_x$), employed to (1) define constitutive relations under stress, (2) determine pressure effects on ductility, and (3) 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

Ann Arbor, MI 48109-2104

305. The Role of Grain Boundary Character in the Environmentally-Assisted Intergranular Cracking Mechanism of Nickel-Base Alloys
G. S. Was, Department of Nuclear Engineering
(313) 763-4675 **01-2**
$143,051

The objective of this program is to determine the role of grain boundary character in the mechamism 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 in both polycrystalline and bicrystalline forms. The ultimate goal is to control grain boundary structure to resist intergranular cracking.

306. The Structural Basis For Fatigue Initiation In Glassy Polymers
A. F. Yee, Department of Materials Science and Engineering
(313) 764-4312 **01-2**
$95,000

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 changes. Relaxation behavior to be used to predict craze initiation.

307. Investigations on the MBE Growth and Properties of AlGaInAs/InP and InGaAs-InAlAs Superlattices
P. K. Bhattacharya, Department of Electrical Engineering and Computer Science
(313) 763-6678
R. Gibala, University of Michigan, Department of Materials and Metallurgical Engineering, Ann Arbor, MI 48109
(313) 763-4970 **01-3**
$14,915 (4 months)

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.

308. A Statistical Mechanics Study of Solid-Solid Interfaces
D. J. Srolovitz, Department of Materials Science and Engineering
(313) 936-1740 **01-3**
$120,000

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.

309. Theory of Non-Equilibrium Growth
L. M. Sander, Department of Physics
(313) 764-4471
R. Savit, Dept. of Physics
(313) 764-3426 **02-3**
$175,218

Theoretical proposal at the forefront of a recent approach to understanding the relationships between growth mechanisms, structure, and properties of non-equilibrium system, 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

310. Micromechanics of Brittle Fracture: Acoustic Emission and Electron Channeling Analyses
W. W. Gerberich, Department of Chemical Eng. and Materials Science
(612) 625-8548 **01-2**
$72,027

Research to address (1) crack dynamics and inherent plasticity effects, (2) ligament contributions to fracture resistance and (3) micro mechanics 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.

311. A Study of Scale Cracking and Its Effects on Oxidation and Hot Corrosion of Metals and Alloys
D. A. Shores, Department of Chemical Engineering and Materials Science
(612) 625-0014 **01-3**
$210,000

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.

312. Modeling and Experimental Studies of Oxide Covered Metal Surfaces TiO_2 on Ti: A Model System
W. H. Smyrl, Chemical Engineering and Materials Science
(612) 625-0717 **01-3**
$450,119

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 electron properties of oxide films investigated by photoelectrochemical microscopy. Calculation of the electron 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 growth and structure of titanium oxide thin films. Determination of the concentration and identity of structural defects in the oxide lattice.

313. Theory of the Electronic and Structural Properties of Solid State Oxides
J. R. Chelikowsky, Department of Chemical Engineering and Materials Science
(612) 625-4837 **02-2**
$50,000

A multi-level theoretical approach to the global properties of solid state oxides will be implemented. The methods which will be applied comprise ab initio pseudopotential calculations, semi-empirical valence force field techniques, and the establishment of empirical chemical "scaling" indices. New computational methods will be developed with emphasis on understanding the nature of the chemical bond arising from oxide formation. The initial systems to be examined are rock salt monoxides, perovskite oxides, and transition metal oxides.

University of Missouri at Columbia
Columbia, MO 65211

314. Inelastic Scattering in Condensed Matter with High Intensity Mossbauer Radiation
W. B. Yelon, Department of Physics
(314) 882-5236 **02-2**
$78,000

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 at Kansas City
Kansas City, MO 64110-2499

315. Theoretical Studies on the Electronics Structure and Properties of Ceramic Crystals and Glasses
W-Y. Ching, Department of Physics
(816) 276-2503 01-1
$127,000

Total energy electronic structure calculations on crystalline and vitreous ceramics. Systematic calculation of electronic and optical properties of high-temperature superconducting oxides. Calculations based on first-principles orthogonalized linear combination of atomic orbitals (OLCAO) method. Development of the excitonic-enhancement model (EEM) of high-temperature superconductivity. Materials studied include superconducting oxides, zirconia, alpha quartz, alumina, silicon nitride, spinel-structured oxides, metallic glasses, and insulating glasses.

University of Missouri at Rolla
Rolla, MO 65401

316. Characterization of Electrically Conducting Oxides
H. U. Anderson, Department of Ceramic Engineering
(314) 341-4886 01-3
$140,000

Interrelationships between electrical conductivity, oxidation reduction kinetics, defect structure, and composition for n- and p-type binary, ternary transition metal oxides, 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 specimen preparation, thermogravimetric characterization, optical microscopy, X-ray and neutron diffraction, TEM, electrical conductivity, Seebeck coefficient studies, thermal and optical stimulated current spectroscopy and deep level transient spectroscopy.

University of Missouri
Columbia, MO 65201

317. High Pressure Optical Studies of Semiconductors and Heterostructures
H. R. Chandrasekhar, Department of Physics and Astronomy
(314) 882-6086 02-2
$59,992

Investigation of the electronic structure, intrinsic and extrinsic, of semiconductors and heterostructures which exhibit electro-optical and magneto-optical properties, using high pressure diamond anvil cell at cryogenic temperatures to tune such properties in a controlled manner. Spectroscopic techniques include photoluminescence, photoreflectance, Raman scattering and excitation spectroscopy. Energies and pressure coefficients of various band extrema and associated defect states determined. Quantum size effects, band movements, discontinuities, and band splitting probed in strained layer superlattices of GaSb-AlSb. Double-well and double-barrier heterostructures studied using electromodulation.

Montana State University
Bozeman, MT 59717

318. Studies of Piezoelectric Polymers
V. H. Schmidt, Department of Physics
(406) 994-6173 03-2
$42,043

Study of chain conformation, rotations, and other motions in the piezoelectric polymers polyvinylidene fluoride and it copolymer with trifluroethylene by NMR and optical techniques. Pressure and temperature dependence on the nonferroelectric to ferroelectric phase transitions. NMR of deutrated 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

319. Fundamental Studies of Strongly Magnetic Rare Earth-Transition Metal Alloys
D. J. Sellmyer, Department of Physics
(402) 472-2407 **02-2**
$59,690

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 sputtering 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

320. Energy Transfer by Triplet Exciton Migration in Polymeric Systems
R. D. Burkhart, Department of Chemistry
(702) 784-6041 **03-1**
$93,200

Studies of triplet-triplet annihilation and rate of triplet exciton diffusion in polymers. Studies of delayed luminescence processes in organic polymers to determine the extend and influence of recombination of geminate ion pairs. 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. Modification of the rate of triplet-triplet annihilation by microwave-induced mixing, monitor the dependence of triplet quantum yields on the energy of excitation, and to probe the direct detection of carbazole radical cations by transient absorption spectroscopy.

University of New Mexico
Albuquerque, NM 87131

321. Radiation Effects and Annealing Kinetics in Crystalline Complex Nb-Ta-Ti Oxides, Phosphates, and Silicates
R. C. Ewing, Department of Geology
(505) 277-4163 **01-1**
$85,000

Investigation of metamict minerals/ion implanted ceramics concerning (1) periodic - aperiodic reaction paths, (2) retained structures in fully damaged materials, and (3) recrystallization products/annealing mechanisms. Techniques include X-ray diffraction, high-resolution transmission electron microscopy (HRTEM), extended X-ray absorption fine-structure spectroscopy (EXAFS), and near-edge spectroscopy (XANES). Materials studied include Ta rich pyrochlores, complex Nb-Ta-Ti oxides, zircon ($ZrSiO_4$), thorite ($ThSiO_4$), monazite ($CePO_4$), titanite ($CaTiSiO_5$), and uraninite (UO_2).

322. Adsorption Studies at a Solid-Liquid Interface
J. A. Panitz, Deparment of Physics
(505) 277-0607 **01-1**
$175,029

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.

City University of New York/City College

New York, NY 10036

323. Investigations of Surface Coatings Based on Silicon and Nitrogen: From Amorphous Si To Silicon Nitride
F. W. Smith, Department of Physics
(212) 690-6963 01-3
$88,000

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, ε_2), IR spectroscopy and core-level spectroscopy. Valence band spectra and binding energy determinations using synchrotron radiation at the BNL NSLS.

324. Dynamics and Pattern Selection at the Crystal-Melt Interface
H. Z. Cummins, Department of Physics
(212) 690-6921 02-2
$104,000

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.

325. Magnetic Properties and Critical Behavior of the Conductivity Near the M-I Transition
M. P. Sarachik, Department of Physics
(212) 690-6904 02-2
$100,000

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 will be undertaken. Focus to be on samples with dopant concentrations near the metal-insulator transition and on just metallic samples which exhibit anomalously strong temperature dependent susceptibilities at low-temperatures. Additional information to be gained by measuring the magnetization as a function of a magnetic field. Low temperature conductivity measurements will determine the exponent in other materials such as Si:B and Si:As.

326. Transport in Small and/or Random Systems
M. Lax, Department of Physics
(212) 690-6864 02-3
$108,000

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 layers in the limit of small size.

City University of New York/Queens College

Flushing, NY 11367

327. Optimization of Film Synthesized Rare Earth Transition Metal Permanent Magnet Systems
F. J. Cadieu, Department of Physics
(718) 520-7463 01-1
$140,000

Synthesis and study of properties of new and potentially useful rare earth transition metal permanent magnet systems. Systems to be examined are the $Nd_2Fe_{14}B$ compound and related compounds, the Sm-Ti-Fe high H_c system, and the $Sm_2(Co,Fe,Zr)_{17}$ type system. Synthesis of a high moment, relatively soft magnetic layer for use in making flux paths and magnetic circuit geometries. Study of sputtering methods that are necessary for synthesis of rare earth and transition metal film systems with highly textured structures. Examination of the steps and procedures required to synthesize adjacent layers of such rare earth and transition metal film systems and to maintain optimum and controlled magnetic properties in the separate layers. Magnetic properties, crystal structures, the role of crystal texturing, and electronic properties will be measured.

State University of New York at Buffalo

Buffalo, NY 14214

328. Construction and Operation of SUNY Facilities at the National Synchrotron Light Source
P. Coppens, Department of Chemistry
(716) 831-3911 02-2
$388,000 (11 months)

Development of facilities at the National Synchrotron Light Source for X-ray diffraction, X-ray absorption spectroscopy, and other X-ray scattering techniques by a participating research team composed of professors from many of the State University of New York campuses, Alfred University, Roswell Park Memorial Institutions, Cortland State College, Geneseo, the University of New Orleans and Allied Corporation. The research interests are: structure of materials, electronic structure of materials, surface physics, compositional analysis, and time-dependent biological phenomena.

State University of New York at Stony Brook

Stony Brook, NY 11794-4466

329. Radiation Embrittlement in BCC Metals
A. H. King, Department of Materials Science & Engineering
(516) 632-8499 01-4
$92,886

Study of 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 with controlled amounts of impurities, particularly carbon, irradiated under various conditions at the High Flux Reactor at Brookhaven National Laboratory. The nature of size distribution of the defect clusters determined by TEM as a function of neutron fluence and impurity content. 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 and unirradiated samples deformed in an electron microscope to observe directly the motion of dislocations and how it is affected as a function of damage parameters. In situ TEM fracture experiments 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. Particular attention to grain boundary fracture.

330. Atomic and Electronic Structure of Metals and Alloys - Clean Surfaces and Chemisorbed Molecules
J. P. Jona, Department of Materials Science and Engineering
(516) 632-8508 02-2
$75,000

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. Research divided into efforts on rare-earth metals, diatomic molecules on metal surfaces, surface and bulk alloys, noble metals and thin films.

331. X-ray Studies of Strin, Interface and Impurity in Semiconductors
Y. H. Kao, Department of Physics
(516) 632-8132 02-2
$85,000

X-ray techniques are employed to pursue a systematic study of short-range-order structure in semiconductors, including strained-layer superlattices, interface in hetrojunctions, 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 measurement making use of synchrotron radiation at NSLS and CHESS.

332. Phase Transition in Polymer Blends and Structure of Ionomers
B. Chu, Department of Chemistry
(516) 246-7792 03-2
$100,000

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 fluroescence, and optical microscopy. Phase separation kinetics measured using 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. Structure of sulfonated polystyrene ionomers using SAXS.

State University of New York at Stony Brook

Stony Brook, NY 11794

333. Theoretical Studies of Chemisorption and Surface Reactions on Nickel and Silicon
J. L. Whitten, Department of Chemistry
(516) 246-6068/5050 03-3
$95,780

Theoretical studies of the adsorption of small molecules and molecular fragments on the surfaces of nickel and silicon using the embedding formulation of ad 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

334. Deposition of A-Si, C:H and A-Si, Ge:H Alloy Thin Films by Remote Plasma Enhanced CVD and Programmable In-situ Etching
W. J. Collis, Department of Electrical Engineering
(919) 334-7760
A. Abul-Fadl, Department of Electrical Engineering
(919) 334-7760 01-5
$65,000

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 State University

Raleigh, NC 27695

335. The Study of Structure-Processing-Property Relations in Copper Oxide-Based High Tc Superconductors
A. I. Kingon, Department of Materials Science and Engineering
(919) 737-7907 01-1
$125,389

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 relationship.

336. Fundamental Aspects of Erosion and Impact Damage
R. O. Scattergood, Department of Materials Science & Engineering
(919) 737-7843 01-5
$92,011

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.

337. Research at and Operation of the Material Science X-ray Absorption Beamline (X-11) at the National Synchrotron Light Source
D. E. Sayers, Department of Physics
(919) 737-2512 **02-2**
$482,124 (11 months)

Development and improvement of beamlines X-11 A and B at the National Synchrotron Light Source, Brookhaven National Laboratory. Transmission, fluorescence electron-yield and X-ray absorption fine structure measurements on a range of materials and interfaces, including metal-semiconductor systems; multilayers and ion implanted layers; electrochemical systems; rare earth metal oxide catalysts; semiconductor alloys; high Tc superconductors; biocatalysts and actinide metals. Development of improved detector systems with spatial resolution. Completion of X-11B optimized for 1 to 8 keV.

338. Band Electronic Structures and Crystal Packing Forces
M. H. Whangbo, Department of Chemistry
(919) 737-3616 **03-1**
$86,700

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

339. Solid-State Voltammetry and Sensors in Gases and Other Non-Ionic Media
R. W. Murray, Department of Chemistry
(919) 962-6295 **03-2**
$125,000

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

340. Momentum Density and Positron Experiments in High-Tc Superconductors
A. Bansil, Department of Physics
(617) 437-2902 **02-3**
$42,330

Quantitative theoretical study concerning the momentum density and electronic structure of high-T_c superconducting compounds and alloys. Existence of the Fermi surface, and adequacy of the local-density (LDA) band theory description of the ground state of $YBa_2Cu_3O_7$ via relevant positron experiments (2D-ACAR). A comprehensive study of the momentum density and its 2D-projections will be carried out along with similar studies of the Bi- and Tl-based compounds. Use of KKR and KKR-CPA and other multiple-scattering theoretic methods, including extensions to accommodate clusters and introduction of newer tools (Such as complex energy integration) to enhance computational efficiency. Calculation of the observable characteristic features of the positron-electron annihilation process, and continuing interactions with experimentalists (including those at BNL, ANL, LLNL) to optimize both theoretical and experimental efforts. Complementary studies of electronic structure and of other processes such as Compton scattering.

Northwestern University
Evanston, IL 60208

341. Defect Clustering and Related Properties of Oxides
J. B. Cohen, Department of Materials Science and Engineering
(312) 491-3665
D. E. Ellis, Department of Physics and Astronomy
(312) 491-3665
T. O. Mason, Department of Materials Science and Engineering
(312) 491-3198 **01-1**
$190,000

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 monoxides (Fe, MnO, CoO, NiO), transition metal spinels (Fe_3O_4 and Mn_3O_4), stabilized ZrO_2, and ternary systems, such as $Ca_xNi_{1-x}O$ and high Tc superconductors. Transport and nonstoichiometry studies in a high oxygen potential cell at oxygen pressures of 1 to 100 atm. which permits substantially higher defect concentrations to be achieved. Structural and valence studies by X-ray and neutron diffraction, electron microscopy, and near-edge absorption spectroscopy. The theoretical effort 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).

342. Nucleation Magnetic Resonance Characterization of Porous Ceramics
W. P. Halperin, Physics and Astronomy Department
(312) 491-3686 **01-1**
$60,000

Application of nuclear magnetic resonance measurements (spin-lattice relaxation and variable-length-scale diffusion) to determine topological nformation on the pore structure of ceramics. Characterization of pore structure in the green state of ceramic materials, such as alumina and silicon carbide, and study of the evolution of the pore structure during sintering. Investigate the relationship between initial pore structure and ultimate density and strength. Study the magnetic alignment of grains in high temperature superconductors and the anomalously enhanced diffusion of liquids in porous ceramics, including xerogel glasses.

343. Ceramic Surfaces and Sintering
L. D. Marks, Dept. of Materials Science & Engineering
(312) 491-3996
D. L. Johnson, Dept. of Materials Science & Engineering
(312) 491-3584 **01-1**
$102,002

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, and 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 coalesce into a macroscopic continuum model.

344. Atomic Structure and Composition of Internal Interfaces
D. N. Seidman, Department of Materials Science and Engineering
(312) 491-4391 **01-1**
$115,058

Atom probe (APFIM) and high-resolution electron microscopy (HREM) studies of metal-ceramic interfaces. Specimens to be prepared by internal oxidation as well as other techniques. Interface structure and composition information to be obtained. Initial studies focussed on Pd/CdO, Pd/NiO and Pd/Al_2O_3 interfaces. Topics of importance include coherency, misfit dislocations, compositional segregation, structure of terminating layers, micro-stoichiometry, dipoles space charge, distribution of point defects and interface impurities.

345. Mechanisms of Transformation Tougening
G. B. Olson, Department of Materials Science and Engineering
(312) 491-2847 **01-2**
$160,000 (10 months)

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 relation for experimental alloys applied to crack-tip and notch fields to study transformation plasticity interaction with various models of microvoid-softening-induced shear localization.

346. Use of Anomalous Small Angle X-ray Scattering to Investigate Microstructural Features in Complex Alloys
J. R. Weertman, Materials Science and Engineering
(312) 491-3537 **01-2**
$98,631

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 Fe_9Cr_1Mo, which has already been examined by small angle neutron scattering. The value of ASAXS as a method of NDE will be investigated.

347. Plasma, Photon, and Beam Synthesis of Diamond Films and Multilayered Structures
R. P. H. Chang, Dept. of Materials Science & Engineering
(312) 491-3598 **01-3**
$85,000

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 reactions, and growth chemistry. Hetero-epitaxial growth of diamond films by a combination of growth techniques in an ultra-high vacuum environment. Investigation of multilayered and superlattice structures of metallic to insulating and semiconducting diamond films. Mass spectroscopy, Auger, and RHEED analysis.

348. Defect Structure of Semiconducting and Insulating Oxides
B. W. Wessels, Department of Materials Sciences and Engineering
(312) 491-3219 **01-3**
$73,000

Characterization of defect structure in doped and electron/proton irradiated epitaxial oxide layers prepared by OMCVD, including electrical compensation by deep level defects, thermal stability of native defects, and electrical/optical characterization of deep level defects. Comparison of theoretically predicted and experimentally determined deep level parameters. Experimental characterization of defect structure by photoluminescence and deep level transient spectroscopies. Materials of interest include ZnO, TiO_2, $SrTiO_3$, and other Ti based perovskites.

349. Energetics, Bonding Mechanism and Electronic Structure of Metal/Ceramic Interfaces
A. J. Freeman, Department of Physics and Astronomy
(312) 491-3644 **02-3**
$103,264

Model the energetics, bonding, bonding mechanism and structure of metal/ceramic interfaces. Investigate surface electronic 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, if appropriate, metal/high T_c superconductor systems. Determine the role of interfacial impurities, such as the irreversible trapping of hydrogen.

350. Mixed Ionic and Electronic Conductivity in Polymers
M. A. Ratner, Department of Physics
(312) 491-5655
D. F. Shriver, Department of Physics
(312) 491-5655 **03-2**
$112,000

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 cathods. 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.

351. Studies of the Structure and Properties of Organic Monolayers, Multilayers and Superlattices
P. Dutta, Department of Physics
(312) 491-5465
J. B. Ketterson, Department of Physics
(312) 491-5468 **03-3**
$104,000

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, and 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.

University of Notre Dame
Notre Dame, IN 46556

352. Single-Electron Charging Effects
S. T. Ruggiero, Department of Physics
(219) 239-7463 **02-2**
$60,000

Charging effects in ultra-small-capacitance metal particles will be studied by electron tunneling, using multiple-barrier tunnel structures of the form metal/barrier/particles/barrier/metal, where the particles are 10-1000 A diameter metal droplets. In concert with preparation of the systems by thin-film deposition and other methods, two types of phenomena are under investigation: (i) competition between intrinsic particle properties and charging effects when the particles are superconducting or magnetic, and (ii) properties associated with irradiation of the systems with 1-10 GHz microwaves. In the latter case, the anticipated phenomena are similar in nature to those caused by the ac Josephson effect in superconducting junctions (Shapiro steps), but which in the present case will originate from charging effects (single-electron tunneling oscillations).

Ohio State University
Columbus, OH 43210

353. Investigations of Ultrasonic Wave Interactions at Imperfect Boundaries Separating Anisotropic Materials
L. Adler, Department of Welding Engineering
(614) 292-1974 **01-5**
$100,000

Fundamental research program on nondestructive characterization of polycrystalline, anisotropic materials. Specific activities 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.

354. The Hydrogen-Induced Stress Corrosion Cracking of Nickel-Base Alloys in High-Temperature Water
P. G. Shewmon, Department of Metallurgical Engineering
(614) 292-5864
S. Smialowska, Department of Metallurgical Engineering
(614) 292-0290 **01-5**
$120,000

Research on the mechanism of the hydrogen-induced intergranular stress corrosion cracking (IGSSC) of Alloy 600, of austenitic Cr-Ni Steels, and of other Ni-containing alloys on exposure to deaerated water at 300-360°C. Determination of the electrochemical conditions under which hydrogen-induced IGSSC occurs in materials of different compositions 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.

355. Theoretical Studies of Dynamics and Correlations in Heavy-Electron Materials
D. Cox, Department of Physics
(614) 292-0620 **02-3**
$44,781

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.

356. Strongly Interacting Fermion Systems
J. W. Wilkins, Department of Physics
(614) 292-5193 **02-3**
$65,000 (6 months)

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-T_c 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.

357. Molecular Ferromagnetism
A. J. Epstein, Department of Physics
(614) 292-1133/3704 **03-1**
$145,400

Study of cooperative magnetic behavior and its microscopic origins in molecular and polymeric materials. Synthesis and characterization of novel ferromagnets and elucidation of the origins of ferromagnetic exchange. Objective is to develop design criteria for the synthesis of new ferromagnetic materials possessing desirable physical properties including high temperature transitions to a ferromagnetic state. 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-tetracyanoquinodimethane (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 ferro-ferrimagnetism. Mossbauer spectroscopy measurements for internal magnetic fields, spectroscopic measurements for charge transfer bands and inelastic neutron scattering measurements for magnetic structure.

Oklahoma State University
Stillwater, OK 74078

358. Rheo-optical Studies of Model "Hard Sphere" Suspensions
B. J. Ackerson, Physics Department
(405) 744-5819 **01-3**
$47,000

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.

359. Radiation Damage of Transition Metal Carbides
C. Y. Allison, Physics Department
(405) 744-5811 **01-4**
$50,000

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

360. Hyperfine Experimental Investigation of Zirconia Ceramics
J. A. Gardner, Department of Physics
(503) 754-3278 **01-1**
$90,000

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-based ceramics that contain either Hf-181 or In-111 as a probe. Investigation of Zr-91 in zirconia by nuclear magnetic resonance (NMR). NQR/NMR experiments to complement and expand the studies of local structure and oxygen vacancy dynamics underway with PAC.

361. Theoretical Studies of Zirconia and Related Materials
H. J. F. Jansen, Dept. of Physics
(503) 754-4631 **01-3**
$59,136

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 97403-0237

362. Surface and Interface Electronic Structure
S. D. Kevan, Department of Physics
(503) 686-4742 **02-2**
$136,840

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.

363. Monitoring Interfacial Dynamics by Pulsed Laser Techniques
G. L. Richmond, Department of Chemistry
(503) 686-4635 **03-2**
$90,000

Studies of interfacial structure and dynamics using second harmonic generation (SHG) and hyper-Raman scattering. Employment of SHG for monitoring electrochemical reactions on a nanosecond to femtosecond time scale, correlation of surface structure with electron transfer kinetics, thin-film nucleation and growth, and analyses of the structure and reactive role of surface defects. Development of novel optical characterization techniques including photothermal deflection, time resolved absorption and luminescence and transient grating spectroscopies.

Pennsylvania State University
University Park, PA 16802

364. Vibrational and Optical Properties of Amorphous Metals
J. S. Lannin, Department of Physics
(814) 865-9231 **01-1**
$95,000

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.

365. The Mechanical Behavior of Surface Modified Ceramics
D. J. Green, College of Earth and Mineral Sciences
(814) 863-2011 **01-2**
$35,000

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.

366. Twin Boundaries, Interfaces and Modulated Structures in Martensites
G. R. Barsch, Materials Research Laboratory
(814) 865-1657 **01-3**
$90,000

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 materials 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.

367. Mass Transfer During Laser Welding
T. DeBroy, Dept. of Materials Science and Engineering
(814) 865-1974 **01-5**
$85,000 (24 months)

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.

368. Topotactic and Epitactic Routes to New Materials
R. Roy, Materials Research Laboratrory
(814) 865-3421
S. Komarneni, Materials Research Laboratrory
(814) 865-1542 **03-2**
$78,830

Synthesis and characterization of crystalline materials formed at low temperatures by topotactic and epitactic routes. 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

369. Structure and Dynamics in Low-Dimensional Guest-Host Solids
J. E. Fischer, Deparment of Materials Science and Engineering
(215) 898-6924 **01-1**
$140,000

Structural and dynamical studies on layer intercalates and doped polymers. Emphasis on competing interactions on phase equilibria, lattice dynamics and microscopic diffusion phenomena in low-dimensional systems. Study of staging phenomenon. X-ray, elastic and inelastic neutron scattering performed as a function of temperature, hydrostatic pressure, doping or intercalate concentration and/or chemical potential. Materials include graphite intercalations (especially with Li and AsF_5), Li-intercalated TiS_2 and alkali-doped polyacetylene.

370. Atomistic Studies of Grain Boundaries in Alloys and Compounds
V. Vitek, Department of Materials Science & Engineering
(215) 898-7883 **01-1**
$115,000

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.

371. Low Stress Brittle Fracture in Polymers
N. Brown, Department of Materials Science & Engineering
(215) 898-8506 **01-2**
$60,000

Research on polyethylene, copolymers and representatives 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.

372. Hardening and Strain Localization in Single and Polycrystalline Materials Under Cyclic Deformation
C. Laird, Department of Materials Science and Engineering
(215) 898-6664
J. L. Bassani, Department of Mechanical Eng. and Applied Mechanics
(215) 898-5632 **01-2**
$150,000

An investigation of latent hardening and strain localization in single crystals under cyclic deformation and modelling 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. The results obtained on cyclically deformed single crystals of various orientations will be used to develop quantitative laws which can be used to predict the behavior of polycrystalline materials. The predictions will be compared to experimental results. In addition to a fundamental understanding of latent hardening and strain localization various manifestations of plastic flow concentrations such as persistent slip bands which appear under cyclic loadings will be studied.

373. Mechanisms of Diffusion Controlled Brittle Fracture
C. J. McMahon, Department of Materials Science & Engineering
(215) 898-7979 **01-2**
$85,000

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 coverage 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.

374. Structure and Vibrational Excitations of Reconstructed Semiconductor Surfaces
E. J. Mele, Department of Physics
(215) 898-3135 **02-3**
$48,684

Theoretical studies of the lattice dynamics of reconstructed semiconductor surfaces. Computations, employing developed theoretical model, will investigate the surface vibration excitations of elemental group IV semiconductors. Application of theoretical methods to relate the microscopic electronic structure of systems to observed structural properties, and ultimately to spectroscopies which can probe structural excitations such as phonons at crystal surfaces and interfaces. Employment of both tight binding total energy methods and state-of-the-art local density methods involving "ab initio" norm conserving pseudopotentials. Electronic and structural properties of As thin films matched to crystalline Si and general study of influence of surface stress on surfaces elastic waves.

University of Pittsburgh
Pittsburgh, PA 15261

375. Microchemical Analysis of Intermetallic Alloys Using the Field-ion Microscope Atom Probe
S. S. Brenner, Department of Metallurgical and Materials Engineering
(412) 624-9738 **01-1**
$105,006

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 substantiated, and comparison between cast and melt-spun materials.

376. Microstructure and Magnetic Properties in High-Energy Permanent Magnets
W. A. Soffa, Department of Materials and Engineering
(412) 624-9728 **01-3**
$124,944

Relationships between microstructures and magnetic properties of permanent magnet alloys. Focus on the polytwinned structures of Fe-Pt, Fe-Pd, and Co-Pt alloys. Control of microstructure through ordering, thermomechanical processing and rapid solidification techniques. Characterization of microstructures by transmission electron microscopy and atom probe field ion microscopy.

377. The Physics of Pattern Formation at Liquid Interfaces
J. V. Maher, Department of Physics and Astronomy
(412) 624-9007 **02-2**
$114,200

Experimental investigation of nonequilibrium phenomena at liquid interfaces. Viscous fingering in rectangular and circular Hele-Shaw cells. Variations of initial conditions to determine transient flow patterns. Saffman-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
Brooklyn, NY 11201

378. Scanning Tunneling Microspectroscopy of Solids and Surfaces
E. Wolf, Department of Physics
(718) 643-2070 **02-2**
$122,000

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.

379. Heavy Fermion and Actinide Materials
P. Riseborough, Department of Physics
(718) 643-5011 **02-3**
$65,532

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 Brehmstrallung isochromat 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 possibly in the new high T_c superconducting oxides.

Princeton University
Princeton, NJ 08544-1033

380. Thermochemistry of Phases Related to Oxide Superconductors
A. Navrotsky, Department of Geological and Geophysical Sciences
(609) 542-4674 **01-3**
$110,000

Investigate the energetics of phases related to oxide superconductors by high-temperature calorimetry. Emphasis on both the energetics of oxidation-reduction reactions involving copper and oxygen and on phase compatibility between superconducting phases and other phases in the multicomponent oxide systems involved. High pressure synthesis (up to 200 kbar) used to explore the full range of oxygen stoichiometry attainable and to synthesize new materials.

381. Control of Microstructure During Consolidation And Injection Modeling of Colloidal Dispersions
W. B. Russel, Department of Chemical Engineering
(609) 452-4590 **01-3**
$75,000

The dynamics of three processes (sedimentation, ultrafiltration, and slip casting) that 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 that 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.

382. Aspects of Photoionization of Impurities and Electron Transfer in Ionic Crystals
D. S. McClure, Department of Chemistry
(609) 452-4980 **03-1**
$105,831

Research on the mechanisms by which impurity ions in host 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

383. X-ray Studies of Laser Annealing in Silicon
R. Colella, Department of Physics
(317) 494-3029 **01-1**
$48,395 (14 months)

Development of theoretical models of disappearance of time resolved diffraction peaks as a result of surface melting of silicon during laser irradiation at the Cornell High Energy Synchrotron Source. Detection of the "photostriction" effect, i.e., contraction of the silicon lattice due to large concentrations of electrons and holes.

384. Materials Research and Beam Line Operation Utilizing NSLS
G. L. Liedl, Materials Engineering Division
(317) 494-4095 **01-1**
$316,000

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, X-ray surface and interface studies.

385. Study of Multicomponent Diffusion and Transport Phenomena
H. Sato, School of Materials Engineering
(317) 494-4096 01-3
$95,000

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.

386. Gamma Scattering in Condensed Matter with High Intensity Mossbauer Radiation
J. R. Mullen, Department of Physics
(317) 494-3031 02-2
$56,000

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 the inelastic scattering, resulting from one phonon processes near the edge of the Brillouin zone.

387. A Study of the Interaction of Light with Sub-Micron Dimensions
R. G. Reifenberger, Department of Physics
(317) 494-3032 02-2
$62,000

Investigation of the photo-excitation 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; photo-excitation 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 semi-conducting and carbide materials. Laser-induced diffusion and desorption effects associated with illumination of adsorbate-covered, submicron surfaces. Exploration of advantages and properties of a laser-illuminated scanning tunneling microscope.

Rensselaer Polytechnic Institute
Troy, NY 12180

388. Mechanism of Mechanical Fatigue in Fused Silica
M. Tomozawa, Department of Materials Engineering
(518) 256-6451 01-2
$95,000

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.

389. Stabilization of High T_c Superconductivity in CdS
R. K. MacCrone, Department of Materials Engineering
(518) 276-6047 01-3
$120,000

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
Houston, TX 77251

390. Studies of Ultrathin Magnetic Films and Particle-Surface Interactions with Spin-Sensitive Electron Spectroscopies
G. K. Walters, Department of Physics
(713) 527-4937
F. B. Dunning, Physics Department
(713) 527-4937 **02-4**
$217,300 (11 months)

Exploitation of spin-sensitive surface spectroscopies to investigate magnetic properties of thin films grown epitaxially on metallic and semiconductor substrates. Artificial materials, prepared as ultrathin films by proper choice of substrate, are grown with different structures and atomic spacing than those obtainable in bulk states. Materials so prepared will be employed to explore quasi-two-dimensional magnetism and complementary fundamental factors which govern magnetism. Spin Polarized Low Energy Diffraction (SPLEED), Metastable Deexcitation Spectroscopy (MDS) and other evolving novel spin-polarized spectroscopic techniques provide required experimental tools.

University of Rochester
Rochester, NY 14627

391. Microstructural Behavior of Non-Equilibrium Systems
J. C. M. Li, Department of Mechanical Engineering
(716) 275-4038 **01-2**
$104,000

Coupled experimental and theoretical research on amorphous metals. Topics include: a) SEMPA examination of amorphous metals with the goal of finding dislocations, b) pulsed dc heating of amorphous metals to improve magnetic properties without annealing embrittlement, c) effect of pulsed dc currents on deformation and annealing of amorphous metals, d) shot peaning and surface oxidation studies to improve mechanical properties, e) studies of magnetic and mechanical properties of nanocrystalline materials, and f) studies of annealing embrittlement through computer simulation of mechanochemical spinodal decomposition.

392. Dynamics of Surface Melting
H. E. Elsayed-Ali, Laboratory for Laser Energetics
(716) 275-5101 03-3
$100,000

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
Thousand Oaks, CA 91360

393. Mechanisms of Mechanical Fatigue in Ceramics
B. N. Cox, Science Center
(805) 373-4128
D. B. Marshall, Science Center
(805) 373-4170
W. L. Morris, Science Center
(805) 373-4545 01-2
$124,958

Investigate the relationship between microstructure and fatigue behavior in fiber/whisker and metal reinforced ceramics. Distinguish crack bridging and crack-tip-shielding mechanisms by very precise measurements of crack opening displacements and displacement fields ahead of the crack tip using a computer-based high accuracy strain mapping system (HASMAP). Study the rate of change of crack bridging forces and the nonlinear constitutive behavior that causes crack shielding. Systematic studies of the effects of variations in microstructure and changes in interface characteristics on fatigue.

Rutgers - The State University
New Brunswick, NJ 08903

394. Research in Two Dimensional Crtical Phenomena and Conformal Field Theory
S. Shenker, Department of Physics
(201) 932-5815
D. Friedan, Department of Physics
(201) 932-5815 **02-3**
$47,000 (3 months)

Research is conducted on a variety of topics. Under investigation are two dimensional critical phenomena and supersymmetric critical phenomena, fluctuating surface models and the associated large N matrix models, string theory, renormalization group flows and the c theorem.

Rutgers - The State University
Piscataway, NJ 08854

395. Multicomponent Glass Surfaces: Structure and Adsorption
S. H. Garofalini, Department of Ceramics
(201) 932-2216 **01-3**
$110,020

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.

SRI International
Menlo Park, CA 94025

396. Fundamental Studies on Passivity and Passivity Breakdown
D. D. Macdonald, Chemistry and Chemical Engineering Laboratories
(415) 859-3195
M. Urquidi-Macdonald, Chemistry & Chemical Engineering Laboratories
(415) 859-3195 **01-3**
$215,022

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.

Seton Hall University
South Orange, NJ 07079

397. Systematic Preparation of Selective Heterogeneous Catalysts
R. Augustine, Department of Chemistry
(201) 761-9033 **03-3**
$72,000

Development of scanning tunneling microscopes to operate in the temperature range 4.2 to 300 K for studies on a wide range of surface atomic structures and electronic phase transitions. The STM will be operated at 4.2 K in magnetic fields, up to 80 kG, to study magnetic field effects on superconductors, magnetic materials, and magnetic field modifications of electronic structures. These studies will include high temperature superconductors, quasi- one and two dimensional metals, semi-metals, semiconductors and intercalated complexes. Special emphasis will be placed on studies of transition metal chalcogenides exhibiting charge-density-wave transitions and showing excellent atomic resolution in the STM.

University of Southern California
Los Angeles, CA 90089

398. Deformation Twinning in Ordered Alloys
E. Goo, Dept. of Materials Science
(213) 743-0961 **01-2**
$74,891

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.

399. Synthesis of Novel Associating Water-Soluble Copolymers
T. E. Hogen-Esch, Department of Chemistry
(213) 743-3798
E. J. Amis, Department of Chemistry
(213) 743-6913 **03-1**
$111,000 (14 months)

Synthesis of water-soluble acrylic and cellulosic copolymers based on perfluorocarbon- and polydimethyl-siloxane derivatives of acrylic comonomers in which the hydrophobe length and that of a flexible polyethylene oxide connecting spacer to the acrylic group are systematically varied. Structural features, important for enhancing the viscosity of aqueous solutions at very low polymer concentrations (ppm), will be investigated with dynamic light scattering, rheology and solution dynamics. The potential for mobility control of water-soluble copolymers that cluster as a result of polyanion-polycation interactions will be explored.

Southwest Research Institute
San Antonio, TX 78284

400. Characterization of Pore Evolution in Ceramics During Creep Failure and Densification
R. A. Page, Department of Materials Sciences
(512) 522-3252
J. Lankford, Department of Materials Sciences
(512) 522-2317 **01-2**
$126,000

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 (using stereo-imaging technique). Cavity size, distribution, morphology, and nucleation and growth rates determined by SANS analysis. Materials investigated included alumina and silicon carbide.

Stanford University
Stanford, CA 94305-6060

401. Mechanical Properties of Materials with Nanometer Scale Microstructures
W. D. Nix, Department of Materials Science and Engineering
(415) 725-2605 **01-2**
$161,853

Study of the mechanical behavior of metals and ceramics with microstructural details as fine as a few nanometers. Materials studied to be produced by multilayer thin film processing techniques and ultra-fine powder processing techniques. Nanoindenter testing used on both types of material. Microbeam and bulge testing also be used on the multilayer films. Transmission electron microscopy and X-ray diffraction to characterize materials of both types.

402. Fundamental Studies of the Chemical Vapor Deposition of Diamond
D. A. Stevenson, Department of Materials Science and Engineering
(415) 723-4251 **01-3**
$115,000

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.

403. A Study of Mechanical Processing Damage in Brittle Materials
B. T. Khuri-Yakub, Department of Electrical Engineering
(415) 723-0718 **01-5**
$92,858

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.

404. A Quest for a New Superconducting State
J. P. Collman, Department of Chemistry
(415) 723-4648
W. A. Little, Department of Physics
(415) 723-4233 03-1
$110,371

Research to understand the mechanism whereby high temperature superconductivity occurs in ceramic cuprates such as $YBa_2Cu_3O_7$ and related substances. A new experimental technique "gap modulation spectroscopy" is being used to study superconducting thin films as prepared by magnetron sputtering, laser ablation or other techniques. Electrochemical experiments using superconducting films as electrodes are under investigation near the superconducting critical temperature T_c. X-ray diffraction results on copper free, superconducting bismuthate materials will be studied above and below T_c searching for a structural phase transition-superconducting mechanism connection. Synthesis of conducting polymer films on superconducting electrode films continues.

University Of Tennessee
Knoxville, TN 37996-1600

405. Statistical Mechanics of Polymer Systems
J. Kovac, Department of Chemistry
(615) 974-3444 03-1
$89,995

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.

406. Investigations of the Effects of Isotopic Substitution and Pressure on Miscribility in Polymer-Polymer and Polymer-Solvent Systems
W. A. Van Hook, Department of Chemistry
(615) 974-5105 03-2
$108,000

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, in particular the consulate 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

407. Fabrication, Phase Transformation Studies, and Characterization of SiC-AlN-Al_2OC
A. V. Virkar, Department of Materials Science and Engineering
(801) 581-5396 01-1
$112,987

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 decompositions, grain boundaries, and the nucleation and growth of grain boundary phases. Establishment of relationship between composition and microstructure to creep behavior and fracture toughness.

408. Alumina Reinforced Tetragonal Zirconia (TZP) Composites
D. K. Shetty, Department of Materials Science and Engineering
(801) 581-6449 01-2
$92,000

Study combined effects of transformation toughening and fiber reinforcement in alumina-zirconia composites. Fabricate, process, and characterize alumina fiber reinforced tetragonal zirconia. 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.

409. Photomodulation Spectroscopy of Photocarrier Dynamics, Electronic Defects and Morphology of Conducting Polymer Thin Films
Z. V. Vardeny, Department of Physics
(801) 581-8372 03-2
$115,000 (18 months)

Study of conducting polymer materials using CW and ultrafast laser spectroscopy. Doped and native polyacetylenes and polythiophenes thin films. Photoexcited electronic states, coupled vibrations, carrier relaxation and recombination processes, resonant Raman spectroscopy. Time-resolved: femtosecond to nanosecond, CW photomodulation spectroscopy, and ultrasonic phonon spectroscopy.

Virginia Commonwealth University
Richmond, VA 23284-2000

410. Electronic Structure and Geometries of Small Compound Metal Clusters
P. Jena, Physics Department
(804) 367-1313
B. K. Rao, Physics Department
(804) 367-1313
S. N. Khanna, Physics Department
(804) 367-1313 01-3
$115,158

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 and states, magnetic moment per atom, binding energies, and ionization potentials of "naked" homo-nuclear clusters using theoretical techniques (with atomic numbers of the constituent atoms as the only input) and by 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

411. Characterization of Superconducting Materials with Muon Spin Rotation
C. E. Stronach, Department of Physics
(804) 520-6153 01-3
$75,000

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

412. Study of the Embedded Atom Method of Atomistic Calculations for Metals and Alloys
R. A. Johnson, Materials Science Department
(804) 924-6356 01-1
$50,000

Use of the Embedded Atom Method of atomistic simulation to provide a greater understanding of the effects of non-central interactions through the use of three-body electron-density functions; alloying interactions using a new form of alloy two-body potential; lattice dynamics, especially including surface phonon effects; and application of the Embedded Atom Method to covalent materials.

413. Initial Stages of Grain Boundary Precipitation
G. J. Shiflet, Department of Materials Science
(804) 924-6340 01-1
$114,000

Studies of the relationship between grain boundary segregation, structure and nucleation/precipitation. Characterization of the active heterogeneous nucleation sites and preferred growth centers at grain boundaries with respect to boundary structure. Techniques include conventional and high resolution electron microscopy as well as high spatial resolution analytical electron microscopy. Five alloy classes selected for study: Al-Mg-Zn, Ti-Cr and Ti-Co, Al-Cu, Co-Fe, and a high-Ni austenitic stainless steel. Theoretical analyses to include segregation thermodynamics and application of models to compute the decrease in grain boundary energy accompanying solute segregation.

414. Surface Structure and Analysis with Scanning Tunneling Microscopy and Electron Tunneling Spectroscopy
R. V. Coleman, Department of Physics
(801) 924-3781 **02-2**
$125,000

Development of scanning tunneling microscopes to operate in the temperature range 4.2 to 300 K for studies on a wide range of surface atomic structures and electronic phase transitions. The STM will be operated at 4.2 K in magnetic fields, up to 80 kG, to study magnetic field effects on superconductors, magnetic materials, and magnetic field modifications of electronic structures. These studies will include high temperature superconductors, quasi- one and two dimensional metals, semi-metals, semiconductors and intercalated complexes. Special emphasis will be placed on studies of transition metal chalcogenides exhibiting charge-density-wave transitions and showing excellent atomic resolution in the STM.

415. Superconducting Materials
J. Ruvalds, Department of Physics
(804) 924-6796 **02-3**
$87,000

Theoretical investigation of the phenomena of superconductivity. High temperature superconductors with Tc 77Kelvin. Alloys, including the Y-Ba-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

416. Metal Induced Embrittlement
R. G. Hoagland, Department of Mechanical & Metallurgical Engineering
(509) 335-8280 **01-2**
$62,000

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 characterized 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

417. Non-Empirical Interatomic Potentials for Transition Metals, Alloys and Semiconductors
A. E. Carlsson, Department of Physics
(206) 543-2778 **02-3**
$82,000

Development of computation 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

418. X-ray and Gamma-Ray Spectroscopy of Solids Under Pressure
R. L. Ingalls, Department of Physics
(206) 543-2778 **02-2**
$112,000

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 Tc superconducting oxides.

419. Fundamental Studies of Elastomers
B. E. Eichinger, Department of Chemistry
(206) 543-1653 **03-1**
$108,000

Chemistry and physics of high 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

420. Electronic and Magnetic Interactions in High Temperature Superconducting and High Coercivity Materials
B. R. Cooper, Department of Physics
(304) 293-3423 02-3
$65,500

Model the interactions between magnetic effects and high temperature superconductivity in the superconducting copper oxides. Investigate the copper-copper magnetic interactions and ordering and the rare earth behavior as a probe of the copper-oxygen electronic system. Examine the basis for the observed praseodymium effect on superconductivity in 123 compounds. Investigate the mechanism of magnetic anisotropy.

University of Wisconsin at Madison
Madison, WI 53706

421. Studies of Alternative-Crystallization-Phase Nucleation
T. F. Kelly, Department of Metallurgical Engineering
(608) 263-1073 01-1
$30,000 (9 months)

This research 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. Studies will address binary Fe-base alloys.

422. Thermodynamics, Kinetics, and Interface Morphologies of Phase Formation Reactions Between Metals and Gallium Arsenide: Bulk vs. Thin-film Studies
Y. A. Chang, Department of Metallurgical and Mineral Engineering
(608) 262-1821 01-3
$110,000

Investigate the thermodynamics, kinetics and interface morphologies of reactions between metals and gallium arsenide in the bulk and thin-film forms. Bulk diffusion-couple measurements of M/GaAs and of thin-film diffusion couples with thin-metal films on GaAs substrates. Bulk samples characterized by optical microscopy, SEM, EPMA and TEM and the thin-film samples primarily by TEM and XTEM and by AES and ESCA. Kinetic data for the bulk samples quantified in terms of ternary diffusion theory. Using the chemical diffusivities obtained from the bulk couples, an attempt will be made to predict the reaction sequences in the thin-film couples. The approach confirmed by its application to a binary metal/silicon system before it is extended to metal/GaAs couples. Rationalize the electrical properties of model-system alloy ohmic contacts to GaAs in terms of the thermodynamic, kinetic and morphological stabilities of these contacts. The initial system a Co-Ge bilayer/GaAs ohmic contact. Electrical characterization and some phase diagram determination. The aim is to provide a basic understand of the electrical properties of alloy/GaAs contacts in terms of their chemical stabilities.

423. Fundamental Studies of New Magnetic Heterostructures: Their Growth, Crystallographic Structure, Magnetic, and Electronic Properties
M. Onellion, Department of Physics
(608) 262-6829 02-2
$99,000

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.

424. Morphological Analysis of Ionomers
S. L. Cooper, Department of Chemical Engineering
(608) 262-1092 **03-2**
$102,630

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 at Milwaukee
Milwaukee, WI 53201

425. Inelastic Electron Scattering from Surfaces
S. Y. Tong, Department of Physics
(414) 229-5765 **02-3**
$93,786

Theory of the inelastic scattering of electron, 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-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 of the University of California at Irvine.

Yale University
New Haven, CT 06520

426. Microstructural Dependence of the Cavitation Damage Function in F.C.C. Materials
B. L. Adams, Department of Mechanical Engineering
(203) 432-4223 **01-2**
$80,000

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

Chronos Research Laboratories, Inc.

4186 Sorrento Valley Blvd
San Diego, CA 91212

427. Radiation Modified Pyroelectric Conversion Materials
R. B. Olsen, Suite H
(619) 455-8200 **Phase II SBIR**
$249,986

The Phase I objective, to establish a novel method for modifying the temperature range over which pyroelectric converter materials can effectively operate, was successfully accomplished. The efforts will proceed to demonstrate high power density and sufficient efficiency for economic pyroelectric conversion. High power density will assure low pyroelectric materials cost (per unit power produced). Efficiency determines the cost of the heat exchangers.

Optra, Inc.

66 Cherry Hill Drive
Berverly, MA 01915

428. Laser Surface Profilometer for Steep Asphric Surfaces
M. Hercher,
(508) 921-2100 **Phase II SBIR**
$248,226

A non-contacting optical sensor for precisely measuring the surface profiles of curved and flat surfaces is being developed. The instrument has already demonstrated excellent height resolution (A), and can handle surface slopes as steep as 10^{o}. Lateral resolution is also excellent (2.5 microns). The instrument is capable of very long and fast scans (no limit on length; speeds up to 25 cm/sec). To facilitate use with steeply curved surfaces, the Laser Profiler is equipped with full autofocus--allowing scans with large dynamic range in terms of height variations (up to 3mm). This combination of features is unique and the proposed instrument will fill a variety of critical needs not presently being met. The use of a laser diode as a source has permited reduced size and cost while at the same time improving ruggedness at no sacrifice in performance. The Phase II instrument will be specificaily configured for inspecting X-ray optics, and will be extensively tested with such surfaces.

Ordela, Inc.

139 Valley Court
Oak Ridge, TN 37830

429. Development of a Method for Greatly Increasing the Count-Rate Capability and Endurance of Position-Sensitive Detector Systems
M. K. Kopp,
(615) 483-8675 **Phase II SBIR**
$416,667

The principal objective of this project is the development of a full-scale production model of a position-sensitive neutron counter system. Based on the results and knowledge gained, this counter system will apply the new technology of charge-centroid measurement developed during the Phase I research to produce an ultra-fast and durable detector system. This system is capable of operating at a count-rate of 105 neutrons per second per pixel and a total count-rate of 107 neutrons per second, a required charge output of only 10 fC per detected neutron, and a spatial resolution of 600 picture elements (pixels). Goals are: (1) design and fabricate the proportional counter, (2) develop a hybrid version of the charge-centroid measurement circuit, (3) instrument a full scale memory and display system, and (4) submit the detector system to extensive tests in neutron-scattering experiments at the High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory.

Advanced Fuel Research, Inc.

87 Church Street
East Hartford, CT 06118

430. Flame Synthesis of Single Crystal Diamond Films
P. W. Monison, Jr.
(203) 528-9806 **Phase I SBIR**
$49,865

The flame CVD method to deposit single crystal diamond films will be defined. A novel flame reactor will be constructed and in-situ diagnostics applied to elucidate the growth chemistry of flame CVD and to improve the film quality. The goal is to demonstrate the deposition of high quality, polycrystalline diamond films covering more than 1 cm^2. Subsequent research will systematically improve the crystallinity and grain size of the films until single crystal growth of diamond is achieved.

Eic Laboratories, Inc.

111 Downey Street
Norwood, MA 02062

431. Low Damage SiC Gratings for Syncrotron Radiation by Photoelectrochemical Etching
M. M. Carrabba
(617) 769-9450 **Phase I SBIR**
$50,000

Diffraction gratings will be fabricated in the surface of chemical vapor deposited (CVD) SiC blanks using photoelectrochemical etching. A goal is to etch patterns projected onto the SiC surface in a one step process, with resolution exceeding 6000 lines/mm. The process will have the advantage of external monitoring and control of the groove uniformity, smoothness and depth. The feasibility of photoelectrochemical etching in n-doped CVD-SiC will be determined, including the demonstration of grating structures using photoresist masks; ultimately direct fabrication of holographic gratings will be sought, with the ultimate goal of producing gratings up to 3" in diameter with a variety of groove spacings and blazes.

Materials Technologies Corporation

57 Maryanne Drive
Monroe, CT 06468

432. Development of High Performance $MoSi_2$/SiC Laminate Composites
Y. Mehrotra
(203) 261-5200 **Phase I SBIR**
$49,895

The main objective of this proposed program is to develop the technology for fabricating high temperature, high oxidation resistant $MoSi_2$/SiC laminated composite structures via a scalable and cost effective chemical vapor deposition (CVD) process. The chemical compatibility between SiC and $MoSi_2$ will be determined at temperatures up to 1650 C. Feasibility of fabricating the laminated structure of the composite will be then be established. Small samples of the composite will be fabricated by deposing alternate layers of SiC and $MoSi_2$ such that large compressive stresses are produced on the composite surface. The composite material will be characterized for important properties such as density, hardness, flexural strength, fracture toughness and thermal expansion coefficient.

Opto-Line Associates, Inc.

15 Stevens Street
Andover, MA 01810

433. Improved Thin Film Multilayer Coatings for Thermal Neutron Guides
J. H. Bradshaw
(508) 470-3275 **Phase I SBIR**
$48,786

Recent developments in multilayer processing and computer simulation of sputter deposition will be extended to supermirror construction suitable for use as large neutron guides. The degree of reflectivity which can be obtained in a single guide wall reflection will be assessed. "Self-leveling" intermetallic compounds and mechanical strain built into the layers themselves will be employed to improve the degree of "flatness" at the atomic level which can be obtained in a multilayer supermirror. Guide segments which test the improvements will be produced.

Ovonic Synthetic Materials Co.

1788 Northwood Dr.
Troy, MI 48084

434. Development of Multilayer Supermirror Coatings from Neutron Guidetubes
J. L. Wood
(313) 362-1290 **Phase I SBIR**
$50,000

Factors impeding the production of reliable supermirrors on a large scale will be investigated. Problems of controlling layer growth and layer uniformity including crystal growth, stress/strain effects, and film/substrate adhesion will be addressed. This research program is directed toward utilizing state-of-the-art deposition process techniques to investigate methods for controlling the layer disturbances on substrates of a limited size. Each method will be evaluated for its success in improving layering quality and neutron reflectivity.

Radiation Monitoring Devices, Inc.

44 Hunt Street
Watertown, MA 02172

435. Position Sensitive Neutron Detector Using Boron Phosphide Semiconductor Sensors
G. Entine
(617) 926-1167 **Phase I SBIR**
$50,000

Traditional position sensitive neutron detectors use either gas filled tubes or scintillator-photomultiplier tube combinations. New position sensitive neutron detectors from solid state detector elements made from the semiconductor boron phosphide (BP) will be constructed. Preliminary work indicates that a new type of thermal neutron detector can be constructed from BP elements. These detectors are very similar to traditional silicon surface barrier detectors used for alpha particle detection. Neutron detection is achieved by detecting the alpha particle produced by the neutron reaction with the boron within the detector. These detectors will be for use in position sensitive detection systems.

Talandic Research Corporation

6042 N. Irwindale Ave.
Irwindale, CA 91706

436. Investigation of High Temperature Superconductor Superlattices Containing Layers of Magnetic or Nonmagnetic Metals
C. Carmichael,
(818) 334-3000 **Phase I SBIR**
$48,733

Current crystal growth techniques can create superlattices in which monolayers of one compound or element are sandwiched between monolayers of another, creating artificial materials, unobtainable by other means. These superlattices are multiple-period structures which do not occur in nature, and possess unusual electron and optical properties. The possibilities of fabricating superlattices containing layers of $YBa_2Cu_3O_{7-x}$ interleaved with layers of either magnetic, or nonmagnetic metals will be investigated. Electron beam evaporation will be used to produce the thin layers in vacuo.

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 beamlines, the NSLS facility has the capacity for running as many as 100 experiments simultaneously.

A total of six insertion devices will ultimately be operating 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, spectro scopy, 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 beamlines constructed by the NSLS staff for general usage, a large number of beamlines 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 beamlines. The conditions and terms are similar to those of the PRTs.

General users are scientists interested in using existing NSLS facilities for experimental programs. General User proposals are reviewed and those accepted are scheduled by an independent beam time allocation committee for a percentage of operating time for each beamline. Liaison and utilization support is provided to the General User by the cognizant beamline.

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. 725D
Brookhaven National Laboratory
Upton, NY 11973

NATIONAL SYNCHROTRON LIGHT SOURCE

TECHNICAL DATA

STORAGE RINGS	KEY FEATURES	OPERATING CHARACTERISTICS
VUV	High brightness; continuous wave length range (λ_c = 25 Å); 17 beam ports	0.75 GeV electron energy
X-ray	High brightness; continuous wave length range (λ_c = 2.5 Å); 30 beam ports	2.5 GeV electron energy

RESEARCH AREA	WAVE LENGTH 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
X-ray Crystallography	0.3 - 6.2	9
X-ray Fluorescence	0.3 - 20	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 = 1.0×10^{15} neutrons/cm^2-sec). The HFBR was designed to provide par ticularly 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 (ϒ >4A). 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_o<$200 MeV Q range: 0.03 $<Q<10_{A-1}$
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 wave-length 4 Å$<\lambda_0<$10 Å
Diffractometer (H3A)	Protein crystallography 20 x 20 cm^2 area detector λo = 1.57 Å
Small Angle Scattering (H3B)	Studies of small angle diffraction of membranes. Double multilayer monochro-mator 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 o<$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 $<E_o<$ 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

R. M. Nicklow — (615) 574-5240
Solid State Division — FTS 624-5240
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6031

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^{2}s at sample (polarized), Vertical magnetic fields to 5 T, Horizontal fields to 2 T, Variable incident energy (E_o)
HB-1A	Triple-axis, fixed E_o, E_o = 14.7 MeV, Wavelength = 2.353 angstroms, Beam size - 5 by 3.7 cm max, Flux - 9 x 10^6 n/cm^{2}s 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^o scattering angle, Flux - 6.8 x 10^5 n/cm^{2}s at sample with 20 min collimation
HB-2, HB-3	Triple-axis, variable E_o, Beam size - 5 x 3.7 cm max, Flux - 10^7 n/cm^{2}s 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^{2}s, 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^{2}s 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^{2}s with 9 min collimation, Curved linear position sensitive detector covering 130^o
HB-4	Correlation chopper, Beam size - 5 x 3.7 cm, Flight path - 1.5 m, 70 detectors covering 130^o, Variable E_o, 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 x 10^{15} n/cm^2 sec. The source has some unique characteristics that have opened up new scientific opportunities:

- high fluxes of epithermal neutrons (0.1-10 eV)
- pulsed nature, suitable for real-time studies and measurements under extreme environment
- white beam, time of flight techniques permitting unique special environment experiments

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, polymers, 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* ($Å^{-1}$)	Range Energy (eV)	Resolution Wave-vector ($Å^{-1}$)	Resolution Energy (eV)
Special Environment Powder Diffractometer (J. D. Jorgensen/K. Volin)	0.5-50	*****	0.35%	*****
General Purpose Powder Diffractometer (J. Richardson/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_o	0.05 E_o
High-Res. Medium-Energy Chopper Spectrometer (D. L. Price)	0.3-9	0-0.4	0.01 k_o	0.02 E_o
Small Angle Diffractometer (J. E. Epperson/ P. Thiyagarajan)	0.006-0.35	*****	.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_o	0.02 E_o
Polarized Neutron Reflect. Neutron Reflect. (POSY II) (G. P. Felcher)	0.0-0.07 0.0-0.25	*****	0.0003 0.001	*****
Quasi-Elastic Neutron Spectrometer (F. Trouw)	0.42-2.59	0-0.1	0.2	0.02 E_o

* Wave-vector, $k = 4\pi \sin\theta/\lambda$.
***** No energy analysis.

<u>INSTRUMENTS NOT YET IN THE USER PROGRAM</u>

eV Spectrometer
Glass, Liquid and Amorphous Materials Diffractometer
(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 diffrac tometer (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
LANSCE Scientific Coordination and Liaison Office
MS H805
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-6069 or
(FTS) 843-6069

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 modifica tions 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 sur faces, 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.

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell
SSRL, Bin 69 PO Box 4349
Stanford, CA 94309-0210

(415) 926-3191
(FTS) 462-3191

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
Oak Ridge National Laboratory — FTS 624-5237
Oak Ridge, Tennessee 37831-6031

J. S. Lin, SAXS-NCSASR — 615) 574-4534
Oak Ridge National Laboratory — FTS 624-4534
Oak Ridge, Tennessee 37831-6031

G. J. Bunick, SANS-NCSASR — (615) 576-2685
Oak Ridge National Laboratory — FTS 626-2685
Oak Ridge, Tennessee 37831-6031

S.Spooner,SANS-NCSASR — (615) 574-4535
Oak Ridge National Laboratory — FTS 624-4535
Oak Ridge, Tennessee 37831-6031

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:	1.5-7.5 m
Beam size at specimen:	0.5-3.0 cm diam
Sample-to-detector distance:	1.5-19 m
Krange:	$2 \times 10^{-3} < K_2 = 4\pi\lambda^{-1} \sin\theta < 0.6$ angstroms $^{-1}$
Detector:	64 by 64 cm^2
Flux at specimen:	10^4-10^6 n/cm^2s 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:	0.2 cm diameter
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 depending on source-sample-detector distances
Detector:	20- by 20-cm^2 (electronic resolution 0.1 by 0.1 cm^2)
Special features:	Time slicing in periods as short as 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 spec trometer (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.

PERSON(S) TO CONTACT FOR INFORMATION

E. A. Ryan	(312) 972-5222
and	FTS 972-5222
N. J. Zaluzec	(312) 972-5075
Electron Microscopy Center for Materials Research	FTS 972-5075
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 A 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 ± 250 eV Current density: H^+, 10 $\mu A/cm^2$ (typical) Ni^+, 3 $\mu A/cm^2$

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

TECHNICAL DATA

Electron Microscopes	Key Features
Texas Nuclear	Terminal voltage 100 kV Energy stability ±300 eV Current density: He^+, 200 μA/cm^2 (typical) Ni+, 2 μA/cm^2
NEC 650 kV Injector Being acquired	Terminal voltage 650 kV Energy stability ± 60 eV Current density: He^+, 100 μA/cm^2 (typical) Ar^+, 10 μA/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 univer sity 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 Metals and Ceramics Division Oak Ridge National Laboratory P. O. Box 2008 Oak Ridge, Tennessee 37831	(615) 574-5066 FTS 624-5066
A. Wohlpart Oak Ridge Associated Universities P. O. Box 117 Oak Ridge, Tennessee 37831	(615) 576-3422 FTS 626-3422

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 120kV	EDS, CBED, STEM; video recording**	Ten 4-h shifts/wk; structural and elemental microanalysis
JEOL 2000FX AEM 200 kV	EDS, CBED, EELS, STEM; examinationof irradiated materials	Ten 4-hr shifts/wk; structural and elemental microanalysis
Philips CM30 AEM 300kV	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 deGraff 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, micro-crystallography, 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.

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.

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

Instruments	"Acronym"	Features and Characteristics
Imaging Secondary Ion Microprobe Cameca IMS 3f	SIMS	Dual ion sources (Cs^{+}, O_2^{+}). 1μm 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
X-ray Photoelectron Spectrometer Physical Electronics 5400	XPS	Resolution: 50 meV, 180° 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	Heating and cooling stages
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 EDX, JEOL JSM 35C (35kV)	SEM	5 nm resolution, channeling and backscattering patterns.
Rutherford Backscattering (in-house construction) (3 MeV)	RBS	Two work stations, channeling
X-ray Equipment Elliott 14 kW high brilliance source Rigaku 12 kW source Several conventional sources	X-ray	4-circle diffractometer. Small angle camera. EXAFS. Lang topography, Powder cameras, etc.

Rigaku D/Max-11B Computer Controlled Powder Diffractometer

CENTER FOR MICROANALYSIS OF MATERIALS

Other Equipment	Acronym	Features and Characteristics
Van de Graff Accelerator for electrons and ions		3 MeV accelerator Rutherford Backscattering Electron radiation damage Ion radiation damage

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	0.1-3.2 MeV; H, O, ^{4}He, ^{3}He, and selected gases. Beam current ~50 microamps
1.7-MV tandem	0.2-3.5 MeV H; 0.2-5.1 MeV ^{3}He, ^{4}He; negative ion sputtering source for heavy ion beams of selected species up to 7 MeV
10-200-KV high-current ion implantation accelerator	Most ion species; 1-3 milliamp singly charged, microamps doubly and triply charged ~100
80-500-kV high-current ion implantation accelerator	Operational in 1990
Lasers	
Pulsed Excimer Laser (0.249 micrometer)	20 x 10^{-9} s; 1.0 joule/pulse
Facilities	
UHV surface and near surface 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; electrical resistivity vs. temperature
Combined ion-beam and laser	Laser and ion beams integrated into processing 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 cover ages 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 available. 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 investi gations 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) Sandia National Laboratories Livermore, California 94551-0969	(415) 294-2697 FTS 234-2697

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.
Linear and Non-Linear Optical Spectroscopy of Electrochemical Systems	Electrochemical cell; Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and diode array detector; Nd:YAG laser, 1 Hz rep. rate.	Electrochemical cell with recirculating pump and nitrogen purge; Monolayer and submonolayer detection of metals, oxygen, and hydrogen adsorption at electrodes.
Nonlinear Optical Spectroscopy of Surfaces System	Picosecond Nd:YAG and dye lasers, 10 Hz; UHV chamber equipped with LEED, Auger, sputtering, and quad. mass spectroscopy; 100-ns pulse length, 10 Hz Nd:YAG laser	Monolayer and submonolayer detection of high temperature hydrogen and oxygen adsorption and nitrogen segregation on alloys; laser thermal disorption
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.
Ultrafast Optical Spectroscopy	Sub-100-fs CPM ring dye laser; copper-vapor-laser-pumped amplifier.	Transient absorption and transient grating experiments.

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_cUpdate, twice-monthly without charge, as both hard copy and electronic mail.

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 characteri zation 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.

MATERIALS PREPARATION CENTER (continued)

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			

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; D. G. Howitt, F. Ponce, J. Barry, C. W. Allen, and L. E. Thomas; internal members are G. Thomas, T. L. Hayes, M. M. Treacy, U. Dahmen, 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,
(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, $\pm 40^\circ$ 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.

SECTION F

Summary of Funding Levels

SUMMARY OF FUNDING LEVELS

During the fiscal year ending September 30, 1989, the Materials Sciences total support level amounted to about $180,746 million in operating funds (budget outlays) and $14,255 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. By Region of the Country

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Northeast (CT, DC, DE, MA, MD, ME, NJ, NH, NY, PA, RI, VT)	37.8	27.0
(b) South (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	13.4	19.4
(c) Midwest (IA, IL, IN, MI, MN, MO, OH, WI)	20.6	26.5
(d) West (AZ, CO, KS, MT, NE, ND,NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	28.2	27.1
	100.0	100.0

SUMMARY OF FUNDING LEVELS (Con't)

2. By Discipline

		Grant Research (% by $)	Total Program (% by $)
(a)	Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01)	58.8	30.6
(b)	Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02)	30.7	28.1
(c)	Materials Chemistry) (Budget Activity Numbers 03	10.5	10.3
(d)	Facility Operations	---	31.0
		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)	32.4
(b)	DOE Laboratory Research Programs	35.3
(c)	Major Facilities at DOE Laboratories	31.0
(d)	Industry and Other	1.3
		100.0

SUMMARY OF FUNDING LEVELS (Con't)

4. By Laboratory and Contract and Grant Research:

	Total Program (%)
Ames Laboratory	4.9
Argonne National Laboratory	15.5
Brookhaven National Laboratory	21.4
Idaho National Engineering Laboratory	0.1
Illinois, University of (Materials Research Laboratory)	2.8
Lawrence Berkeley Laboratory	8.6
Lawrence Livermore National Laboratory	0.8
Los Alamos National Laboratory	5.7
Oak Ridge National Laboratory	16.8
Pacific Northwest Laboratory	1.3
Sandia National Laboratory	3.6
Solar Energy Research Institute	0.1
Stanford Synchrotron Radiation Laboratory	1.0
Contract and Grant Research	17.4
	100.0

SECTION G

Index of Investigators, Materials, Techniques, Phenomena, and Environment

Investigator Index

Investigator Index

Investigator Index

Investigator Index

Investigator Index

Investigator Index

Investigator Index

Investigators Index

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 1989 were $180,746,000. The number of projects is 434.

MATERIALS

Actinides-Metals, Alloys and Compounds

6, 15, 32, 34, 35, 52, 127, 129, 138, 139, 144, 151, 173, 208, 225, 355, 356, 379
(1.08, 0.80, 4.15)

Aluminum and its Alloys

7, 18, 42, 63, 67, 70, 75, 78, 86, 107, 108, 111, 129, 142, 156, 169, 199, 205, 219, 222, 235, 249, 252, 264, 267, 312, 336, 373, 414
(1.54, 0.81, 6.68)

Alkali and Alkaline Earth Metals and Alloys

4, 42, 58, 173, 253, 293
(0.28, 0.31, 1.38)

Amorphous State: Liquids

39, 94, 99, 117, 180, 201, 265, 268, 282, 323, 325, 377, 404
(0.65, 0.71, 3.00)

Amorphous State: Metallic Glasses

19, 24, 29, 53, 66, 67, 88, 107, 116, 135, 141, 151, 156, 161, 169,
190, 201, 214, 275, 316, 340, 364, 391
(1.29, 1.55, 5.30)

Amorphous State: Non-Metallic Glasses (other than Silicates)

30, 35, 71, 83, 16 190, 201, 202, 203, 218, 243, 278, 282, 322, 324, 329, 334, 403
(0.76, 1.15, 4.15)

Amorphous State: Non-Metallic Glasses (Silicates)

16, 35, 81, 138, 139, 185, 189, 201, 203, 223, 278, 282, 316, 329, 364, 388, 395
(1.08, 1.19, 3.92)

Carbides

16, 71, 73, 105, 129, 131, 132, 139, 140, 165, 166, 171, 177, 179, 203, 218, 219, 252, 266, 267, 336, 342, 343, 359, 399, 406, 429
(1.50, 1.08, 6.22)

Carbon and Graphite

107, 122, 169, 198, 216, 266, 369, 382, 428
(0.65, 0.16, 2.07)

Coal

162
(0.05, 0.07, 0.23)

Composite Materials--Structural

13, 26, 88, 105, 139, 140, 157, 169, 183, 203, 211, 266, 267, 302, 336, 349, 407, 430
(0.78, 0.57, 4.15)

Copper and its Alloys

1, 3, 5, 9, 13, 28, 42, 49, 65, 79, 87, 104, 111, 123, 131, 142, 171, 199, 200, 209, 235, 238, 242, 270, 272, 303, 304, 335, 362, 372, 373, 424
(1.98, 1.21, 7.37)

Dielectrics

14, 16, 83, 88, 121, 165, 166, 198, 243, 248, 289, 348
(0.48, 0.34, 2.76)

Fast Ion Conductors (use Solid Electrolytes if more appropriate)

30, 35, 42, 88, 165, 202, 248, 296
(0.41, 0.51, 1.84)

Iron and its Alloys

1, 2, 3, 5, 7, 15, 41, 49, 53, 65, 74, 75, 79, 80, 86, 87, 106, 108, 109, 111, 124, 129, 142, 151, 154, 155, 156, 158, 161, 184, 186, 198, 206, 209, 211, 213, 235, 244, 249, 250, 255, 259, 263, 267, 286, 290, 293, 297, 300, 306, 311, 320, 345, 346, 354, 367, 373, 376, 384, 396, 416, 419, 424
(4.38, 2.44, 14.52)

Glasses (use terms under Amorphous State)

136, 139, 140, 165, 282, 342, 350, 395
(0.41, 0.43, 1.84)

Nickel and its Alloys

4, 5, 19, 24, 41, 49, 53, 65, 67, 70, 74, 78, 79, 87, 142, 156, 161, 169, 177, 184, 198, 199, 217, 219, 222, 226, 236, 249, 252, 255, 259, 263, 264, 297, 300, 302, 306, 312, 333, 353, 354, 375, 384
(2.07, 1.67, 9.91)

Nitrides

16, 20, 21, 37, 105, 129, 132, 165, 179, 187, 203, 219, 316, 324, 343, 402, 406
(0.81, 0.72, 3.92)

Oxides: Binary

20, 25, 26, 30, 33, 36, 39, 51, 54, 58, 71, 82, 83, 85, 105, 106, 113, 114, 129, 130, 132, 145, 156, 157, 165, 180, 193, 203, 204, 211, 218, 243, 251, 251, 252, 255, 259, 266, 285, 288, 293, 297, 305, 312, 313, 316, 317, 322, 324, 336, 341, 342, 343, 348, 360, 361, 365, 381, 384, 399, 407
(2.93, 2.36, 14.06)

Oxides: Non-Binary, Crystalline

20, 25, 28, 32, 33, 50, 54, 81, 82, 92, 106, 108, 113, 114, 126, 138, 139, 146, 154, 156, 165, 176, 179, 180, 193, 203, 208, 217, 243, 248, 252, 253, 257, 260, 266, 274, 285, 288, 289, 294, 295, 296, 305, 317, 322, 335, 341, 348, 354, 360, 378, 410
(2.72, 2.06, 11.98)

Polymers

16, 21, 43, 56, 60, 89, 93, 96, 97, 100, 128, 145, 148, 149, 151, 162, 169, 182, 183, 188, 207, 210, 231, 232, 233, 262, 277, 283, 307, 319, 321, 329, 332, 339, 350, 351, 369, 371, 403, 404, 417, 422, 425
(2.65, 2.03, 9.91)

Platinum Metal Alloys (Platinum, Palladium, Rhodium, Irridium, Osmium, Ruthenium)

12, 26, 69, 95, 107, 111, 129, 132, 199, 245, 256, 270, 287, 420
(0.46, 0.47, 3.23)

Quantum Fluids and Solids

13, 30, 35, 52, 94, 115, 116, 122, 147, 161, 216, 224, 265, 281, 382
(1.11, 0.89, 3.46)

Radioactive Waste Storage Materials (Hosts, Canister, Barriers)

81, 208, 322, 368
(0.32, 0.06, 0.92)

Structural Ceramics (Si-N, SiC, SIALON, Zr-O (transformation toughened))

21, 23, 66, 73, 77, 79, 83, 85, 105, 107, 139, 140, 151, 152, 153, 157, 160, 179, 180, 203, 207, 257, 288, 299, 305, 316, 324, 342, 343, 360, 361, 365, 399, 402, 406
(2.14, 1.44, 8.06)

Surfaces and Interfaces

1, 2, 13, 15, 18, 23, 29, 31, 34, 35, 40, 42, 43, 48, 52, 55, 56, 58, 63, 66, 68, 69, 70, 71, 75, 78, 91, 92, 101, 102, 105, 107, 112, 113, 114, 117, 119, 122, 123, 124, 128, 132, 137, 139, 140, 149, 151, 154, 155, 156, 157, 160, 164, 175, 177, 178, 179, 180, 183, 185, 186, 187, 188, 189, 193, 194, 196, 198, 199, 201, 203, 205, 212, 228, 229, 232, 238, 241, 249, 251, 255, 256, 259, 263, 275, 283, 287, 288, 291, 299, 303, 304, 305, 308, 309, 312, 323, 325, 329, 331, 333, 337, 339, 343, 351, 353, 362, 363, 365, 370, 385, 390, 395, 401, 407, 409, 421, 431, 432
(7.67, 8.76, 27.42)

Synthetic Metals

38, 60, 149, 210, 277, 301, 338
(0.55, 0.42, 1.61)

TECHNIQUES

Electron Energy Loss Spectroscopy (EELS)

1, 16, 23, 24, 32, 67, 68, 70, 73, 101, 107, 109, 110, 113, 132, 152, 153, 177, 194, 203, 204, 220, 221, 242, 256, 284, 287, 308, 387, 423
(1.73, 1.49, 6.91)

Elastic Constants

25, 31, 86, 142, 246, 266, 289, 353, 366
(0.37, 0.24, 2.07)

Electrochemical Methods

23, 38, 39, 41, 60, 65, 99, 100, 117, 123, 124, 125, 129, 131, 165, 173, 179, 184, 186, 192, 193, 247, 248, 271, 287, 290, 304, 339, 350, 354, 363, 396, 420, 429
(1.91, 1.30, 7.83)

Electron Microscopy (technique development for all types)

2, 3, 5, 8, 24, 26, 37, 48, 67, 68, 70, 71, 73, 75, 77, 78, 84, 87, 107, 108, 109, 110, 111, 113, 126, 135, 137, 138, 139, 140, 140, 142, 149, 52, 153, 156, 157, 158, 159, 167, 172, 178, 203, 204, 226, 228, 235, 237, 256, 263, 264, 283, 287, 288, 293, 294, 305, 322, 323, 330, 335, 341, 343, 354, 359, 376, 407
(4.08, 3.42, 15.44)

Electron Spectroscopy for Chemical Analysis (ESCA)

22, 31, 33, 42, 58, 71, 72, 75, 101, 105, 132, 139, 140, 186, 299
(0.51, 0.56, 3.46)

Electron Spin Resonance or Electron Paramagnetic Resonance

40, 82, 113, 116, 166, 192, 195, 248, 301, 389
(0.37, 0.53, 2.30)

Extended X-Ray Absorption Fine Structure (EXAFS and XANES)

22, 25, 33, 34, 48, 49, 60, 71, 81, 125, 132, 138, 139, 151, 201, 208, 248, 322, 329, 331, 337, 416
(1.04, 1.55, 5.07)

Field Emission and Field Ion Microscopy

23, 26, 69, 152, 153, 194, 323, 375
(0.35, 0.40, 1.84)

High Pressure (Technique development of all types)

12, 30, 41, 121, 144, 145, 146, 180, 195, 305
(0.39, 0.48, 2.30)

Ion or Molecular Beams

24, 42, 43, 66, 72, 113, 146, 156, 160, 167, 174, 176, 178, 196, 209, 214, 227, 270
(0.76, 1.02, 4.15)

Ion Channeling, or Ion Scattering (including Rutherford and other ion scattering methods)

24, 27, 29, 42, 66, 68, 75, 78, 113, 126, 156, 160, 166, 174, 175, 178, 190, 206, 227
(1.04, 1.90, 4.38)

Internal Friction (also see Ultrasonic Testing and Wave Propagtion)

86, 248, 257, 289, 366
(0.14, 0.01, 1.15)

Infrared Spectroscopy (also see Raman Spectroscopy)

40, 41, 82, 118, 120, 126, 132, 145, 149, 165, 167, 189, 190, 202, 207, 242, 248, 277, 289, 296, 299, 308, 317
(0.88, 0.72, 5.30)

Laser Spectroscopy (scattering and diagnostics)

42, 43, 100, 120, 121, 128, 136, 145, 149, 167, 180, 183, 191, 193, 196, 197, 198, 229, 247, 278, 318, 319, 321, 325, 332, 363, 377, 392, 402, 422, 426
(1.77, 0.94, 7.14)

Magnetic Susceptibility

6, 12, 13, 25, 31, 32, 38, 51, 116, 133, 144, 146, 147, 168, 176, 192, 195, 225, 273, 295, 301, 326, 355, 376
(1.61, 1.40, 5.53)

Molecular Beam Epitaxy

31, 72, 90, 92, 113, 191, 197, 206, 226, 234, 276, 308, 331
(0.55, 0.33, 3.00)

Mossbauer Spectroscopy

32, 40, 108, 213, 214, 295, 315, 357, 386, 416
(0.58, 0.29, 2.30)

Neutron Scattering: Elastic (Diffraction)

11, 14, 30, 38, 39, 40, 52, 53, 54, 59, 94, 98, 144, 146, 148, 161, 162, 163, 164, 176, 182, 234, 265, 266, 268, 282, 296, 341, 364, 369, 404, 426, 427
(1.38, 2.80, 7.60)

Neutron Scattering: Inelastic

11, 30, 39, 40, 52, 53, 59, 94, 98, 161, 162, 163, 164, 182, 234, 265, 289, 357, 364, 366, 404, 426, 427
(1.06, 2.46, 5.30)

Neutron Scattering: Small Angle

30, 40, 98, 131, 148, 162, 164, 182, 283, 399, 404, 426, 427
(0.44, 1.39, 3.00)

Nuclear Magnetic Resonance and Ferromagnetic Resonance

12, 40, 82, 95, 115, 116, 126, 128, 132, 148, 192, 202, 207, 216, 248, 277, 283, 342, 360, 382, 413
(1.43, 0.73, 4.84)

Optical Absorption

15, 23, 33, 40, 102, 126, 136, 149, 187, 191, 285, 321
(0.44, 0.36, 2.76)

Perturbed Angular Correlation and Nuclear Orientation

360, 361
(0.12, 0.02, 0.46)

Photoluminescence

16, 99, 100, 136, 146, 191, 237, 258, 278, 308, 334, 348
(0.51, 0.26, 2.76)

Positron Annihilation (including slow positrons)

55, 60, 63, 307, 340
(0.28, 0.20, 1.15)

Powder Consolidation (including sintering, hot pressing, dynamic compaction, laser assisted, etc., of metals and ceramics, use this item in the Phenomena index)

8, 9, 28, 51, 54, 83, 85, 105, 112, 141, 146, 157, 168, 173, 183, 257, 286, 296, 320, 342, 343, 419
(1.31, 0.92, 5.07)

Surface Treatment and Modification (including ion implantation, laser processing, electron beam processing, sputtering, etc., see Chemical Vapor Deposition)

29, 40, 42, 58, 65, 67, 70, 105, 108, 112, 113, 132, 135, 136, 139, 140, 156, 160, 164, 165, 167, 168, 174, 175, 178, 179, 186, 190, 191, 212, 218, 227, 237, 284, 287, 299, 324, 331, 334, 350, 352, 365, 383, 429, 431, 432, 434
(2.81, 2.86, 10.83)

Synthesis

20, 21, 22, 28, 38, 40, 54, 60, 71, 77, 89, 92, 93, 96, 97, 126, 128, 129, 132, 146, 148, 149, 179, 180, 183, 188, 192, 195, 210, 219, 225, 262, 286, 295, 299, 320, 368
(2.97, 1.84, 8.53)

Theory: Defects and Radiation Effects

27, 36, 50, 63, 66, 134, 138, 139, 156, 170, 186, 200, 208, 218, 228, 248, 260, 318, 322, 348, 359, 383
(1.36, 1.56, 5.07)

Theory: Electronic and Magnetic Structure

6, 19, 22, 25, 33, 35, 36, 40, 41, 47, 57, 91, 104, 122, 126, 129, 136, 137, 144, 149, 154, 170, 191, 192, 200, 203, 231, 276, 295, 313, 316, 327, 340, 355, 356, 357, 361, 374, 379, 409, 411, 413, 418
(2.53, 1.74, 9.91)

Theory: Non-Destructive Evaluation

7, 212, 353
(0.23, 0.11, 0.69)

Theory: Surface

36, 42, 47, 57, 69, 84, 91, 114, 122, 125, 126, 132, 154, 170, 221, 228, 233, 238, 275, 276, 294, 309, 333, 339, 343, 349, 351, 370, 374, 395, 409, 411, 423
(1.84, 1.16, 7.60)

Theory: Structural Behavior

4, 6, 18, 49, 94, 104, 105, 108, 122, 148, 149, 157, 159, 189, 200, 205, 211, 236, 246, 249, 250, 253, 255, 257, 266, 276, 289, 305, 306, 309, 311, 312, 319, 335, 336, 338, 345, 349, 351, 361, 366, 369, 371, 372, 373, 391, 399, 402, 409, 414, 415, 422
(3.43, 1.80, 11.98)

Theory: Superconductivity

17, 28, 32, 35, 50, 57, 91, 115, 116, 122, 126, 144, 146, 154, 170, 176, 192, 295, 316, 338, 355, 356, 389, 410, 413, 418
(1.64, 1.36, 5.99)

Theory: Thermodynamics, Statistical Mechanics, and Critical Phenomena

39, 47, 57, 91, 94, 103, 104, 108, 116, 126, 128, 129, 141, 142, 147, 148, 157, 167, 170, 180, 181, 182, 200, 223, 230, 231, 238, 241, 246, 249, 253, 265, 275, 291, 309, 339, 366, 385, 403, 417, 424
(2.07, 1.50, 9.45)

Theory: Transport, Kinetics, Diffusion

2, 3, 25, 40, 50, 65, 66, 69, 103, 108, 123, 124, 131, 154, 156, 164, 165, 167, 170, 180, 191, 213, 217, 218, 223, 230, 231, 236, 248, 257, 260, 275, 296, 299, 310, 316, 327, 339, 341, 350, 361, 367, 374, 377, 379, 381, 385, 396, 419
(2.56, 2.40, 11.29)

Thermal Conductivity

8, 147, 164
(0.35, 0.86, 0.69)

Ultrasonic Testing and Wave Propagation

7, 65, 224, 248, 353, 366, 402
(0.53, 0.19, 1.61)

Vacuum Ultraviolet Spectroscopy

15, 34, 46, 58, 125
(0.21, 0.37, 1.15)

Work Functions

42, 117
(0.09, 0.05, 0.46)

X-Ray Scattering and Diffraction (wide angle crystallography)

8, 14, 20, 22, 25, 26, 31, 33, 34, 37, 38, 54, 56, 60, 81, 94, 98, 105, 113, 119, 123, 126, 128, 133, 135, 138, 139, 141, 142, 145, 148, 151, 155, 171, 182, 198, 206, 226, 227, 235, 237, 243, 254, 259, 262, 263, 266, 282, 286, 293, 296, 302, 308, 312, 317, 320, 322, 328, 329, 341, 348, 365, 369, 389, 406, 420
(3.23, 2.33, 15.21)

X-Ray Scattering (small angle)

31, 81, 125, 148, 151, 169, 189, 201, 214, 283, 307, 329, 332, 334, 346, 383, 417
(0.76, 1.17, 3.92)

X-Ray Scattering (other than crystallography)

14, 30, 34, 46, 56, 125, 151, 155, 182, 201, 272, 293, 315, 328, 331, 351, 384, 386
(0.99, 1.61, 4.15)

X-Ray Photoelectron Spectroscopy

20, 22, 25, 41, 46, 48, 58, 60, 78, 101, 113, 125, 132, 177, 185, 189, 201, 242, 304, 324, 329, 395
(0.92, 1.73, 5.07)

PHENOMENA

Dynamic Phenomena

35, 36, 52, 116, 117, 121, 147, 161, 162, 163, 170, 182, 186, 188, 193, 198, 221, 232, 247, 270, 275, 278, 289, 310, 315, 332, 366, 377, 381, 384, 386, 392, 423
(2.00, 1.65, 7.60)

Electronic Structure - Metals including amorphous forms 1, 15,

19, 20, 22, 32, 34, 35, 55, 58, 90, 95, 107, 117, 122, 126, 129, 137, 144, 146, 154, 170, 201, 213, 214, 245, 286, 316, 320, 337, 340, 352, 356, 362, 374, 379, 413, 421
(1.91, 2.28, 8.76)

Electronic Structure - Non-metals including amorphous forms

19, 25, 33, 55, 71, 72, 90, 99, 117, 122, 146, 200, 231, 246, 273, 278, 316, 318, 326, 327, 335, 339, 348, 362, 383, 415
(1.43, 0.69, 5.99)

Erosion

336
(0.00, 0.00, 0.23)

Grain Boundaries

2, 5, 8, 26, 37, 48, 49, 51, 63, 75, 78, 83, 105, 107, 113, 137, 142, 152, 153, 154, 156, 159, 171, 172, 184, 198, 199, 203, 205, 251, 255, 257, 258, 263, 264, 286, 288, 291, 294, 303, 306, 309, 320, 335, 349, 353, 354, 373, 375, 384, 399, 406, 424
(2.30, 1.94, 12.21)

Hydrogen Attack

73, 74, 75, 78, 145, 190, 209, 306, 354
(0.51, 0.27, 2.07)

Ion Beam Mixing

24, 27, 29, 42, 66, 113, 156, 160, 174, 175, 179, 214, 218
(0.76, 1.71, 3.00)

Laser Radiation Heating (annealing, solidification, surface treatement)

42, 65, 72, 109, 136, 145, 167, 171, 174, 175, 190, 275, 383, 392
(0.81, 1.26, 3.23)

Mechanical Properties and Behavior: Fracture and Fracture Toughness

5, 7, 25, 28, 74, 77, 78, 79, 80, 105, 108, 109, 139, 140, 145, 156, 157, 159, 211, 250, 252, 263, 266, 267, 293, 304, 305, 307, 311, 322, 330, 336, 345, 365, 371, 373, 391, 399, 402, 406, 407, 414
(1.80, 1.00, 9.68)

Materials Preparation and Characterization: Ceramics

20, 28, 33, 50, 54, 73, 83, 92, 105, 107, 109, 112, 114, 126, 138, 139, 146, 152, 153, 157, 169, 176, 179, 180, 189, 202, 207, 219, 228, 243, 251, 252, 257, 274, 278, 285, 288, 294, 296, 299, 305, 317, 324, 335, 343, 348, 359, 365, 368, 381, 388, 399, 401, 406, 407
(2.70, 1.80, 12.67)

Materials Preparation and Characterization: Glasses

34, 107, 135, 139, 141, 166, 189, 202, 212
(0.32, 0.37, 2.07)

Materials Preparation and Characterization: Metals

2, 3, 9, 13, 14, 20, 24, 37, 42, 54, 66, 92, 103, 107, 108, 109, 111, 123, 129, 131, 133, 135, 137, 142, 145, 152, 153, 159, 166, 169, 173, 206, 212, 214, 219, 225, 226, 238, 252, 264, 286, 293, 320, 354, 389, 391
(2.07, 1.91, 10.60)

Materials Preparation and Characterization: Polymers

60, 89, 93, 96, 97, 128, 132, 148, 149, 182, 183, 283, 307, 332, 339, 351, 404
(0.69, 0.63, 3.92)

Materials Preparation and Characterization: Semiconductors

14, 16, 90, 92, 107, 113, 133, 191, 197, 212, 227, 237, 258, 271, 274, 308, 318, 331, 334, 347, 348, 420
(1.24, 0.62, 5.07)

Nondestructive Testing and Evaluation

5, 7, 132, 212, 346, 353
(0.30, 0.20, 1.38)

Phonons

4, 11, 13, 19, 52, 64, 88, 98, 118, 120, 121, 122, 161, 162, 163, 170, 212, 221, 223, 246, 249, 253, 270, 284, 289, 366, 374, 387, 423
(1.73, 1.29, 6.68)

Recrystallization and Recovery

81, 94, 108, 175, 247, 302, 322, 372
(0.65, 0.30, 1.84)

Residual Stress

7, 266, 365, 402
(0.21, 0.06, 0.92)

Rheology

85, 128, 189, 196
(0.23, 0.33, 0.92)

Stress-Corrosion

41, 49, 65, 74, 184, 186, 304, 306, 313, 354, 388
(0.69, 0.49, 2.53)

Solidification (conventional)

2, 9, 158, 216, 229, 230, 244, 247, 325, 367, 382
(0.46, 0.27, 2.53)

SOL-GEL Systems

82, 139, 140, 157, 169, 176, 189
(0.46, 0.50, 1.61)

Solidification (rapid)

2, 30, 63, 67, 135, 170, 175, 230, 295, 297, 376
(0.51, 0.65, 2.53)

Surface Phenomena: Chemisorption (binding energy greater than 1eV)

1, 15, 43, 58, 90, 95, 101, 102, 114, 117, 122, 123, 124, 130, 131, 132, 154, 177, 204, 209, 220, 221, 233, 242, 275, 281, 287, 308, 323, 329, 333, 343, 351, 362, 363, 390, 397, 412, 423
(2.03, 1.18, 8.99)

Surface Phenomena: Physiosorption (binding energy less than 1eV)

18, 31, 42, 56, 58, 59, 101, 117, 118, 132, 177, 194, 216, 220, 308, 343, 351, 363, 382, 387, 395
(1.11, 1.05, 4.84)

Surface Phenomena: Structure

13, 18, 34, 36, 40, 69, 84, 92, 95, 102, 117, 118, 119, 122, 123, 132, 155, 170, 177, 184, 199, 204, 221, 238, 241, 256, 259, 270, 272, 304, 309, 323, 329, 331, 340, 343, 349, 351, 365, 374, 383, 384, 395, 397, 412, 415, 423
(2.90, 1.50, 10.83)

Surface Phenomena: Thin Films (also see Coatings in this index)

30, 31, 33, 34, 37, 40, 46, 48, 58, 71, 72, 90, 100, 101, 113, 117, 120, 122, 123, 124, 125, 132, 141, 160, 178, 179, 187, 193, 194, 196, 198, 204, 206, 212, 216, 221, 232, 238, 247, 256, 276, 308, 312, 313, 324, 328, 347, 349, 352, 364, 382, 390, 396, 401, 421, 423, 428, 431, 432, 433, 434
(3.99, 3.25, 14.06)

Short-range Atomic Ordering

34, 117, 132, 154, 155, 182, 183, 185, 188, 200, 213, 235, 351, 364, 397, 412
(0.92, 0.77, 3.69)

ENVIRONMENT

Aqueous

41, 65, 82, 85, 117, 119, 123, 124, 128, 184, 185, 188, 189, 204, 232, 247, 290, 304, 306, 313, 323, 351, 354, 368, 396
(4.22, 3.11, 5.76)

Gas: Hydrogen

5, 26, 73, 75, 78, 106, 118, 130, 145, 193, 198, 199, 281, 306, 401
(2.05, 1.59, 3.46)

Gas: Oxidizing

26, 78, 105, 145, 146, 159, 193, 198, 204, 219, 220, 250, 284, 285, 297, 312, 324
(1.41, 1.20, 3.92)

Gas: Sulphur-Containing

198, 287, 297, 312
(0.41, 0.17, 0.92)

High Pressure

12, 14, 19, 41, 52, 53, 54, 99, 121, 127, 132, 145, 146, 163, 164, 191, 217, 225, 246, 254, 360, 369, 416
(2.33, 3.23, 5.30)

Magnetic Fields

6, 12, 17, 25, 28, 32, 45, 50, 52, 53, 59, 108, 116, 127, 134, 146, 149, 163, 168, 225, 234, 308, 326, 328, 413
(2.70, 4.14, 5.76)

Radiation: Electrons

86, 87, 110, 115, 134, 138, 139, 204, 218, 287, 348, 359, 387
(1.41, 1.45, 3.00)

Radiation: Gamma Ray and Photons

14, 34, 38, 42, 45, 46, 134, 136, 138, 139, 155, 164, 186, 218, 278, 318, 329
(1.77, 3.86, 3.92)

Radiation: Ions

42, 43, 66, 138, 139, 146, 156, 160, 168, 174, 175, 190, 208, 214, 227, 273, 322, 348
(2.58, 3.30, 4.15)

MAJOR FACILITIES: OPERATIONS

Pulsed Neutron Sources (Operations)

44, 143, 150
(0.69, 5.88, 0.69)

Steady State Neutron Sources (Operations)

61, 164
(0.46, 12.45, 0.46)

Synchrotron Radiation Sources (Operations)

34, 62, 119
(0.69, 7.71, 0.69)