DOE/ER-0295
Dist. Category UC-25

September 1986

Materials Sciences Programs

Fiscal Year 1986

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 organizational structure of the Department of Energy is given in an accompanying chart. The Office of Basic Energy Sciences reports to the Director of the DOE 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 multipurpose laboratories under the jurisdiction of the Department, excluding laboratories 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, Biological Energy Research, Engineering and Geosciences, Advanced Energy Projects, and Carbon Dioxide Research Divisions. Materials Sciences research is supported primarily at DOE National Laboratories and Universities. The research covers a spectrum of scientific and engineering areas of interest to the Department of Energy and is conducted generally by personnel trained in the disciplines of Solid State Physics, Metallurgy, Ceramics, Chemistry, and Materials Science. The structure of the Division is given in an accompanying chart.

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

This report contains a listing of research underway in FY 1986 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.

Louis C. Ianniello, Acting Director
Division of Materials Sciences
Office of Basic Energy Sciences

RECENT DIVISION SPONSORED PUBLICATIONS

Topical and Workshop Reports[a]

- Final Report the Workshop on Conductive Polymers (1985)
- Micromechanisms of Fracture (1985)
- Polymer Research at Synchrotron Radiation Sources (1985)
- Bonding and Adhesion at Interfaces (1985)
- Corrosion-Resistant Scales in Advanced Coal Combustion Systems (1985)
- Novel Methods for Materials Synthesis (1984)[c]
- Theory and Computer Simulation of Materials Structures and Imperfections (1984)
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Coatings and Surface Modifications (1983)[c]
- High Pressure Science and Technology (1982)
- Scientific Needs of the Technology of Nuclear Waste Containment (1982)
- Radiation Effects (1981)
- Condensed Matter Theory and the Role of Computation (1981)
- Research Opportunities in New Energy-Related Materials (1981)[c]
- Aqueous Corrosion Problems in Energy Systems (1981)[c]
- High Temperature Corrosion in Energy Systems (1981)[c]
- Basic Research Needs and Opportunities on Interfaces in Solar Materials (1981)[c]
- Basic Research Needs on High Temperature Ceramics for Energy Applications (1980)[c]

Summary Research Bulletins (of Work in Progress)[a]

- Ceramic Processing
- Non-Destructive Evaluation
- Sulfur Attack
- Welding

Description of Research Facilities, Plans, and Associated Programs

- Centers for Collaborative Research[a]
- Materials Sciences Division - Long Range Plan (1984)[a]
- Progress of the Office of Energy Research (1985)[a]

---

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

[b] To be published.

[c] Also published in Materials Science and Engineering.

OFFICE OF BASIC ENERGY SCIENCES
Division of Materials Sciences Structure

Division of Materials Sciences

Acting Director: L. C. Ianniello

(Sandy Tucker-Secretary)
(301) 353-3427

Metallurgy and Ceramics Branch

Chief: F. V. Nolfi, Jr.

(Taree Thompson-Secretary)
(301) 353-3428

R. J. Gottschall
J. B. Darby
D. W. Keefer 1/

Solid State Physics and Materials Chemistry Branch

Chief: B. C. Frazer

(Kathy Rockenhauser-Secretary)
(301) 353-3426

T. A. Kitchens 2/
I. L. Thomas
J. E. Robinson 3/
W. T. Oosterhuis 4/
D. Liebenberg 5/

Notes:

1/ On Detail from Idaho National Engineering Laboratory (returned 9/86)
2/ Relocated to Applied Mathematical Sciences, DOE, 9/86
3/ On Detail from Argonne National Laboratory
4/ On Leave from National Science Foundation (returned to NSF 8/86)
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 six sections. Section A contains all Laboratory projects, Section B has all contract research projects, Section C has projects funded under the Small Business Innovation Research Program, Sections D and E have information on DOE collaborative research centers, Section F gives distribution of funding, and Section G has various indexes.

Each project in Sections A, B, and C carries a number (at the left hand margin) for reference purposes, e.g., in Section G. The FY 1986 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), or Materials Chemistry (03). 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 - Chemical Structure
03-2 - Engineering Chemistry
03-3 - High Temperature and Surface Chemistry

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 a number of selected categories. Most projects have been classified under more than one category since the categories are not mutually exclusive. 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 1986 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 the Division's secretaries: S. Tucker, T. Thompson, and K Rockenhouser. Computer programming assistance was provided by S. Dorsey, Calculon, Inc.

TABLE OF CONTENTS

SECTION A - LABORATORIES

SECTION B - Grant and Contract Research

SECTION C - Small Business Innovation Research

SECTION D - Major User Facilities

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

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

Metallurgy and Ceramics - 01 -

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

001. MATERIALS SCIENCE OF INTERFACES

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

$145,000 01-1

Studies of interface structure and composition using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Auger and reflection electron loss spectroscopy of metallic hydrides for phase identification and mapping. Effects of tin alloying on brass corrosion behavior in aqueous salt solutions. Scanning Auger microprobe analysis (350) of effects of radiation on the competition between C and P grain boundary segregation in iron. Local chemical state information from Auger lineshape analysis in metallic glasses.

002. SURFACES AND SOLIDIFICATION

R. K. Trivedi, J. T. Mason, V. K. Seetharaman
Phone: (515) 294-5869

$290,000 01-1

Theoretical and experimental studies of the effect of temperature gradient, growth rate and composition on the stability and steady-state shape of solid-liquid interfaces obtained during controlled solidification. Study of morphological transition from dendritic to cellular to eutectic structure. Experimental work on primary dendrite spacing, eutectic spacing and interface structures in Pb-Sn, Pb-Au, Pb-Pd and Pb-Bi systems. Study of interface stability and morphological characteristics in model transparent material such as succinonitrile and acetone mixture. Microstructure development during amorphous to crystalline transition.

AMES LABORATORY (continued)

003. MICROSTRUCTURAL CONTROL IN METALS

J. D. Verhoeven, A. R. Pelton, R. W. McCallum, E. D. Gibson, F. C. Laabs
Phone: (515) 294-9471

$580,000 01-1

Production of composite alloys by the in situ process and properties of in situ prepared Cu-base composite alloys. Problems in the diffusion of Sn and Ga to form Nb_3Sn and Nb_3Ga. Directional solidification studies on segregation and morphology in gray, nodular, and white cast iron. Evaluation of microstructural changes in the austempering of nodular cast irons. Microstructure evolution under solidification conditions typical of welding processes. Solidification processing of $(Dy,Tb)Fe_2$ magnetostrictive alloys. Processing and characterization of high coercivity, permanent magnet materials.

004. MECHANICAL METALLURGY

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

$460,000 01-2

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Interstitial effects on strength and ductility in both nonhydrogenated and hydrogenated V, Nb, and Ta. Investigation of hydrogen diffusion in vanadium-base alloys by internal friction. Hydrogen-induced brittle cracking in both low and high hydrogen solubility bcc metals and alloys. Effects of radiation-induced defects and solute segregation on 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.

005. STRUCTURE AND PROPERTY RELATIONS IN METALS

J. F. Smith
Phone: (515) 294-5083

$6579,000 01-3

Thermodynamic functions in Y-Fe, Y-Co, and Y-Ni systems from electromotive force measurements. Computer analysis of thermodynamic data for the prediction of stable and metastable phase equilibria, metallic glass formation, and control of microstructures. Ultrasonic measurements of stress and texture in solids.

AMES LABORATORY (continued)

006. TRANSPORT STUDIES

O. N. Carlson
Phone: (515) 294-2375

$135,000 01-3

Study of fast diffusion and electrotransport of iron, cobalt and nickel in scandium and thorium. Determination of activation energies, mechanism and defect responsible for fast diffusion. Thermotransport and diffusion of interstitial solutes in vanadium-titanium and vanadium-niobium alloys. Determination of solid solubility of interstitial solutes in vanadium.

007. HYDROGEN IN METALLIC SOLIDS

D. T. Peterson
Phone: (515) 294-6585

$170,000 01-3

Diffusion, thermotransport, and solubility of H and D in V alloys with Ti, Nb, Al or O. Photoelectron spectroscopy, and metallography of metal hydrides and solid solutions of H in vanadium-base alloys. Local mode energies for hydrogen in metals and metallic solids.

008. RARE EARTH MATERIALS

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

$210,000 01-3

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

AMES LABORATORY (continued)

009. NDE MEASUREMENT TECHNIQUES

O. Buck, R. B. Thompson, C. V. Owen, D. K. Rehbein, D. C. Jiles
Phone: (515) 294-3930
$552,000 01-5

Techniques to measure failure-related material properties to improve understanding of failure mechanisms and inspection reliability. Ultrasonic measurement of internal stresses, texture, and porosity. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide information about closure near crack tip and its influence on crack growth rate and detectability. Microscopic characterization and modeling of the effects of stress and deformation on crack initiation and growth in brass under corrosive conditions. Relationship between fatigue damage or stress and magnetic properties.

010. ADVANCED MATERIALS AND PROCESSES

F. A. Schmidt, O. D. McMasters
Phone: (515) 294-5236 or (515) 294-1562
$189,000 01-5

New process for high-purity vanadium. Development of melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys. Alternative processes for preparing rare earth-iron alloys and for producing oriented crystallites of magnetostrictive compounds. Processing of stoichiometric and non-stoichiometric materials by an inducively coupled plasma. Electrotransport and zone melting for maximum purification of rare earth and refractory metals. Processing of single crystals of congruent melting and peritectic materials by levitation zone melting, free-standing vertical zone melting, Bridgman, Czochralski and strain-anneal recrystallization. Above research being conducted in the Materials Preparation Center described in the Section-Collaborative Research Centers.

AMES LABORATORY (continued)

Solid State Physics - 02 -

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

011. NEUTRON SCATTERING

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

$337,000 02-1

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

012. SEMICONDUCTOR PHYSICS

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

$225,000 02-2

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

013. SUPERCONDUCTIVITY

D. K. Finnemore, J. R. Ostenson, E. L. Wolf, T. P. Chen
Phone: (515) 294-3455

$460,000 02-2

Point contact Josephson effect in heavy fermion superconductors UBe_{13}, $CeCu_2Si_2$. Electron tunneling spectroscopy and surface physics studies of strong coupled transition metal superconductors. Proximity electron tunneling spectroscopy (PETS) of the electron-phonon spectrum ^{2}F( ). Auger electron spectroscopy (AES), electron energy loss spectroscopy (ELS) and ultraviolet photoemission spectroscopy (UPS). Fundamental studies of superconductivity in metal-metal composites, use of Josephson junctions to study flux pinning of isolated vortices, development of materials with very low pinning, development of superconducting composites suitable for large scale magnets in the 8 to 16 Tesla range, practical studies to improve wire fabrication techniques, development of magnetic shielding devices, study of magnetostrictive materials.

AMES LABORATORY (continued)

014. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS

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

$315,000 02-2

Electron photoemission and optical properties (transmission, reflection, ellipsometry, electroreflectance) of solids in the visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation. Ce and Ce-compounds (e.g., $CeSn_3$) heavy Fermion systems, e.g., UPt_3, Fe-based alloys with Si and Al, benzotriazol on Cu, electroreflectance of emersed Ag electrodes, photon- and electron-stimulated desorption of neutral atoms from insulators.

015. NEW MATERIALS AND PHASES

R. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson,
P. Klavins, D. R. Torgeson
Phone: (515) 294-5435

$570,000 02-2

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

AMES LABORATORY (continued)

016. MATERIALS FOR HYDROGEN STORAGE

R. G. Barnes, K.-M. Ho, D. T. Peterson, C. Stassis
Phone: (515) 294-4754 or (515) 294-1560
$70,000 02-2

Multiprogram effort focused toward understanding hydrogen and other interstitial-metal interactions. Phase diagram studies of ternary systems (e.g., Nb-O-H, Y-O-H). The solubility limits of interstitials in alloys (e.g., H in BnB-v, v-tI). Interstitial-interstitial interactions (trapping effects). Modification of interstitial diffusion by other interstitials. Interstitial effects on lattice vibrational behavior and mechanical properties. Influence of interstitials on electronic structure. Experimental approaches include thermodynamics and kinetics, specific heat, elastic and inelastic neutron scattering, XPS, UPS, and Auger spectroscopy, NMR, embrittlement and mechanical properties. Band theoretical methods are applied to electronic structure and diffusion.

017. X-RAY DIFFRACTION PHYSICS

J.-L. Staudenmann, D. S. Robinson
Phone: (515) 295-3585 or 294-9614
$200,000 02-2

X-ray diffraction studies of semiconducting compounds, epitaxial layers, and superlattices as a function of the temperature. In-situ diffusion studies between layers in superlattices. X-ray studies of La at high pressures. X-ray Debye temperature and electron charge density studies of V_3Si and Fe-Ni-C in the vicinity of the martensitic phase transition. Active participation in the MATRIX PRT beam line at NSLS.

018. ELECTRONIC AND MAGNETIC PROPERTIES

B. N. Harmon, K.-M. Ho, M. Luban, C. T. Chan, C. Soukoulis, J. Luscombe
Phone: (515) 294-7712
$438,000 02-3

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

AMES LABORATORY (continued)

019. OPTICAL AND SURFACE PHYSICS THEORY

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

$100,000 02-3

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

020. SUPERCONDUCTIVITY THEORY

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

$130,000 02-3

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

021. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS

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

$444,000 03-1

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

AMES LABORATORY (continued)

022. CERAMIC MATERIALS

T. J. Barton, L. E. Burkhart, G. Burnet, M. J. Murtha
Phone: (515) 294-8074
$425,000 03-2

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

023. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS

H. F. Franzen
Phone: (515) 294-5773
$150,000 03-3

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

AMES LABORATORY (continued)

024. ELECTRONIC AND MAGNETIC PROPERTIES

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

$449,000 03-3

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

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

K. L. Kliewer - Phone (FTS) 972-3570 or (312) 972-3570

Metallurgy and Ceramics - 01 -

F. Y. Fradin - Phone (FTS) 972-4925 or (312) 972-4925
H. Wiedersich - Phone (FTS) 972-5079 or (312) 972-5079

040. DEFECTS IN ALLOYS

R. W. Siegel, R. Benedek, J. E. Robinson, L.C. Smedskjaer, Z. Li, T. Lu.
Phone: (312) 972-4963

$518,000 01-3

A fundamental research program concerned with the atomic and electronic structure of defects in alloys and the relationship between these and the properties of stable and metastable phases and the nature of phase transformations. The research program involves investigations of defect properties and atomic and electronic structure in a variety of materials, with an emphasis on disordered and ordered alloy systems. These materials are being investigated with experimental techniques such as positron annihilation spectroscopy, Compton scattering, X-ray and neutron scattering, and transmission electron microscopy, along with complementary electronic structure calculations.

041. DEFECTS IN CERAMICS

D. J. Lam, K. L. Merkle, J. N. Mundy,
J. L. Routbort, D. Wolf
Phone: (312) 972-4966

$849,000 01-3

Theory of defect kinetics and atomic structure in grain boundaries. TEM studies of atomic configurations in grain boundaries in oxides. Grain boundary diffusion in metal oxides. Diffusion mechanisms and impurity interactions in mixed alkali germanate, alkali-alumino-germanate, and alkali-silicon-sulfur glasses. Diffusion mechanisms and point defect studies in transition metal oxides as a function of oxygen partial pressure at high temperature using cation and oxygen tracer diffusion, conductivity, and TEM techniques. Effect of nonstoichiometry and defect clustering on mechanical deformation of oxides. Preparation of single crystals and bicrystals of metal oxides.

ARGONNE NATIONAL LABORATORY (continued)

042. IRRADIATION AND KINETIC EFFECTS

L. E. Rehn, R. S. Averback, R. C. Birtcher, M. A. Kirk, N. Q. Lam, B. A. Loomis, P. R. Okamoto, H. Hahn, F.-R. Ding, A. Liu
Phone: (312) 972-5021

$1,268,000 01-4

Investigations of mechanisms leading to the formation of defect aggregates, precipitates, and other inhomogeneous distributions of atoms in solids with and without displacement-producing irradiation. Surface layer modification of alloys by ion implantation, ion-beam mixing, and sputtering. Radiation-induced segregation to internal and external defect sinks. Radiation-enhanced diffusion. Effects of irradiation on alloy composition, microstructure, and amorphization. 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. Analytical electron microscopy. Radiation sources include HVEM-2MV Tandem facility and two 300-kV ion accelerators.

043. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

H. Wiedersich, C. W. Allen, A. Taylor, N. J. Zaluzec
Phone: (312) 972-5079

$1,329,000 01-4

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, and gaseous environments. Ion-beam interface with 300 kV ion accelerator and 2 MV tandem accelerator available for in-situ implantations and irradiations. A 600 kV ion accelerator is being procured as a replacement for the 300 kV instrument. Approximately 50% of HVEM usage is by non-ANL scientists on research proposals approved by the Steering Committee for the Center that meets every six 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 lower-voltage conventional electron microscopes.

ARGONNE NATIONAL LABORATORY (continued)

044. OXIDATION STUDIES

D. J. Lam, D. J. Baxter, W. E. King, K. Natesan, S. J. Rothman
Phone: (312) 972-4966

$763,000 01-5

Cation and anion transport processes in pure and doped protective-oxide material using tracer diffusion and secondary-ion mass spectrometry techniques. Impurity ion location, adhesion and morphology of oxide scales on Y- and Zr-doped Fe-Cr and Fe-Cr-Ni alloys using analytical electron microscopy and HVEM techniques. Mechanisms and kinetics of oxide film breakdown in bioxidant atmospheres. Deformation properties of alloy-scale composite systems. Scale microcracking and decohesion observed by acoustic emission techniques. X-ray photoelectron spectroscopic studies of the chemical aspects of scale development and breakdown.

045. AMORPHOUS METALLIC ALLOYS

P. R. Okamoto, R. S. Averback, T. I. Morrison, H. Hahn
Phone: (312) 972-5052

$581,000 01-5

Investigations of the synthesis of amorphous metallic materials by isothermal solid-state reactions at the interfaces of vapor-deposited multilayer films and mixed metal powders, by ion-beam mixing of multilayer films, and by displacement damage of intermetallic compounds by electron and ion beams. Tracer diffusion measurements in amorphous alloys. In-situ high-voltage electron microscopy studies of the morphology and kinetics of the crystalline-to-amorphous transformations. The effect of irradiation on diffusion, segregation, and crystallization of amorphous alloys. Investigations of the relationship between the atomic structure of amorphous alloys and their magnetic and superconducting properties. Synthesis of ultra-fine metallic powders. Materials characterization methods include X-ray diffraction, electron microscopy, electrical resistivity, Rutherford backscattering, AES, EELS, and EXAFS.

ARGONNE NATIONAL LABORATORY (continued)

Intense Pulsed Neutron Source Division

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

046. INTENSE PULSED NEUTRON SOURCE PROGRAM

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

$4,762,000 02-1

Operation and development of IPNS, an intermediate-flux pulsed spallation neutron source for condensed matter research with neutron scattering and irradiation techniques. The facility is equipped with 6 instruments which are regularly scheduled for users and 5 beam tubes which are for special experiments or developing instruments. The facility has been run since 1981 as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 200 experiments, involving about 100 outside visitors from universities and other institutions are performed annually. Industrial Research on a proprietary basis, which allows the company to retain full patent rights, has been initiated with a number of companies (e.g., Schlumberger-Doll, Amoco, Sohio, Ontario Hydro) and is encouraged. Relevant Argonne research programs appear under the neutron activities of the Materials Science and Technology Division of Argonne National Laboratory.

Solid State Physics - 02 -

F. Y. Fradin - Phone (FTS) 972-4925 or (312) 972-4925
M. B. Brodsky - Phone (FTS) 972-5016 or (312) 972-5016

047. NEUTRON AND X-RAY SCATTERING

D. L. Price, T. O. Brun, J. E. Epperson, J. Faber, G. P. Felcher,
J. D. Jorgensen, S. Susman, R. O. Hilleke, U. Walter
Phone: (312) 972-5475

$1,726,000 02-1

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

ARGONNE NATIONAL LABORATORY (continued)

048. SUPERCONDUCTIVITY AND MAGNETISM

B. D. Dunlap, G. W. Crabtree, K. E. Gray, D. G. Hinks,
H. A. Kierstead, T. I. Morrison, G. K. Shenoy, E. Alp, A. J. Fedro,
S. K. Malik, P. A. Montano, B. D. Terris
Phone: (312) 972-5538

$1,312,000 02-2

Experimental and theoretical investigations of the magnetic and superconducting properties of materials. Studies of ternary compounds including Chevrel phase and rare-earth rhodium boride materials. Electronic and transport studies of organic superconductors. Studies of the electronic properties of mixed valence, heavy fermion and other narrow-band materials containing rare-earth and actinide elements. Studies of amorphous superconductors. Soft X-ray synchrotron beam-line development. Experimental techniques include the de Haas-van Alphen effect, Mossbauer spectroscopy, transport and magnetic measurements, electron tunneling, EELS, NMR, EXAFS and XANES, heat capacity, materials preparation, and characterization.

049. ELECTRONIC STRUCTURE AND BONDING

D. J. Lam, A. T. Aldred, S.-K. Chan, M. V. Nevitt,
B. W. Veal
Phone: (312) 972-4966

$897,000 02-2

Experimental and theoretical studies of electronic structure and its relationship to physical and chemical properties and bonding in solids. X-ray photoemission (XPS) and X-ray absorption (XANES and EXAFS) spectroscopic studies of structural and electronic properties of multicomponent oxygen compounds. Crystal chemistry and structural phase transformation studies of complex metal oxides using X-ray diffraction and electron microscopy. Thermal and lattice properties study of ABO_4 compounds using heat capacity, EXAFS, Raman scattering and ultrasonic measurements. Theoretical studies of photoelectron spectra and bonding of ABO4 compounds and stabilized cubic zirconia. Development of molecular cluster code to calculate total energy of embedded oxide clusters. Formulation of the theory of EXAFS and XANES for multicomponent systems.

ARGONNE NATIONAL LABORATORY (continued)

050. LAYERED AND THIN FILM MATERIALS

I. K. Schuller, S. D. Bader, M. B. Brodsky, M. Grimsditch,
E. Moog
Phone: (312) 972-5469

$697,000 02-2

Research on the growth and physical properties obtained by thin film techniques--epitaxial films and sandwiches, metallic superlattices, amorphous metals, and superconductors. Preparation techniques include molecular beam epitaxy, and evaporation. Materials characterization methods include X-ray scattering, low- and high-energy electron diffraction, for structural studies. Low temperature transport, superconductivity, and magnetism. Electronic structure studies via AES, UPS, and XPS in conjunction with theoretical band structures. Elastic, magnetic, and vibrational properties using Brillouin and Raman scattering.

051. SYNCHROTRON RADIATION STUDIES

G. K. Shenoy, A. J. Arko, S. D. Bader, G. S. Knapp, A. R. Krauss,
D. Y. Smith, M. G. Strauss, B. W. Veal Jr., C. E. Young
Phone: (312) 972-5537

$985,000 02-2

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

ARGONNE NATIONAL LABORATORY (continued)

052. LOW DIMENSIONAL AND INTERFACE MATERIALS

I. K. Schuller, P. Roach, Y. Lepetre, K. Yang, H. Homma, M. Schneider
Phone: (312) 972-5469

$307,000 02-2

Research on the properties of interfaces and low dimensional materials. Monolayers, superlattices, and epitaxial films are being prepared by molecular beam epitaxy and sputter deposition. Characterization is performed using high- and low-energy electron diffraction, X-ray and neutron diffraction, X-ray photoelectron and Auger spectroscopy. Physical properties are being studied using low temperature magnetotransport and magnetic measurements. Growth phenomena and interfacial structure are being studied using Molecular Dynamics simulation.

053. 6GeV SYNCHROTRON SOURCE RESEARCH AND DEVELOPMENT

Y. Cho
Phone: (312) 972-6616

$834,000 02-2

Preconstruction R&D work including further refinement of ideas, firming up the construction techniques proposed in the Conceptual Design Report, particularly these incoming new ideas and hi-tech items. Continuing dialogue with the user community concerning the user support plans for the facility. Two categories of R&D: one mainly concerned with accelerator design and construction parameters, and the other with beam lines and experimental facilities. Schedule planned so that construction would start in FY88. Current estimate of construction period is 4 1/2 yrs.

054. CONDENSED MATTER THEORY

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

$900,000 02-3

Condensed matter theory in statistical physics, electronic band structure, many body effects, amorphous materials, and the defect solid state. Molecular-dynamics modeling of defect mediated phase transitions and multicritical behavior, and of atomic and molecular glasses. Electronic structure calculations of narrow-band metal and alloy systems. Simulation of quantum systems by Monte Carlo methods. Mesoscopic physics (localization in wires). Spatial and electronic structure of covalent glasses. Clusters. Transport in ionic conductors. Electronic structure by simulated annealing. The systems studied include molten salts, ternary superconductors, rare earth and actinide compounds, multilayers, and SiO_2 and chalcogenide glasses.

ARGONNE NATIONAL LABORATORY (continued)

055. MODELING AND THEORY OF INTERFACES

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

$161,000 02-3

Computer simulation of the physical properties of interphase boundaries between dissimilar materials, involving both atomistic simulation methods (lattice statics and dynamics, molecular dynamics, Monte-Carlo) and electronic structure calculations. The latter are aimed at deriving two- and three-body interatomic potentials as well as calculating certain relatively simple bulk and defect properties directly (i.,e., without assumption of potentials). The atomistic simulations are used to determine, for example, the structure and free energy of solid interfaces as 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 interfaces between them.

056. ULTRA-HIGH FIELD SUPERCONDUCTORS

K. E. Gray, R. T. Kampwirth, D. W. Capone II
Phone: (312) 972-5521

$298,000 02-5

Development of magnetron sputtered films of superconducting NbN for use in magnets operating in the 15-24 Tesla range. Effort includes effect of preparation conditions and substrate type on superconducting properties such as critical current density and upper critical field. Radiation and strain tolerance. Material characterization by X-ray, SEM and TEM. Coating of sputtered NbN films with copper stabilizer. Coating of wires and both sides of tapes. Technique development for fabrication of continuous tapes and/or wires suitable for winding ultra-high field superconducting magnets.

ARGONNE NATIONAL LABORATORY (continued)

Materials Chemistry - 03 -

F. Y. Fradin - Phone (FTS) 972-4925 or (312) 972-4925
D. M. Gruen - Phone (FTS) 972-3513 or (312) 972-3513

057. CHEMICAL AND ELECTRONIC STRUCTURE

J. M. Williams, M. A. Beno, C. D. Carlson, A. J. Schultz,
H. H. Wang, R. J. Thorn, T. J. Emge, U. Geiser, P. C. W. Leung
Phone: (312) 972-3464
$2,010,000 03-1

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

058. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

M. Blander, R. A. Blomquist, L. A. Curtiss, V. A. Maroni,
M.-L. Saboungi, S. VonWinbush
Phone: (312) 972-4548
$501,000 03-2

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

ARGONNE NATIONAL LABORATORY (continued)

059. INTERFACIAL MATERIALS CHEMISTRY

D. M. Gruen, V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, M. H. Mendelsohn, M. J. Pellin, M.-K. Ahn
Phone: (312) 972-3513

$626,000 03-2

Complementary fundamental research activities that focus on the structural, electronic, and catalytic properties of macro-molecular systems such as zeolites and transition metal clusters. Studies of new transition metal-containing zeolites by extended X-ray absorption fine structure, electron paramagnetic resonance, nuclear magnetic resonance, Mössbauer, and infrared spectroscopies, as well as by high-voltage electron microscopy, neutron inelastic scattering spectroscopy and ab initio molecular orbital theory, with the aim of elucidating the relationship between zeolite structure and catalytic activity/selectivity. Examinations of ligand-free transition metal clusters formed in low-temperature rare gas matrices by time resolved laser fluorescence, laser Raman, optical-optical double resonance, excited state absorption spectroscopy, and X-ray absorption fine structure methods to gain knowledge of the bonding properties and molecular/electronic structure of metal cluster systems. Ab initio molecular orbital calculations, alone or in combination with statistical mechanical analyses, on polynuclear metal clusters and on molecule/surface interactions in zeolite-like environments that yield incisive knowledge of adsorbate-substrate interactions on a molecular level.

060. AQUEOUS CORROSION

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

$628,000 03-2

Basic research aimed at elucidating fundamental aspects of aqueous corrosion at high temperature and pressure (300°C and 10 MPa) with emphasis on mechanisms responsible for stress corrosion cracking of iron- and nickel-based alloys. Studies of the details connecting surface adsorption, surface reaction, film formation, electrolyte chemistry effects, and grain boundary processes with crack initiation and propagation using a combination of in situ surface sensitive spectroscopic methods and transient electrochemical techniques. Ambient and high-temperature studies of processes occurring at corrodent metal-electrolyte interfaces and concurrent research directed towards testing corrosion models. Investigations of the structure of oxide films on metal surfaces in aqueous media using synchrotron radiation sources. In situ measurements using laser-Raman scattering Raman-gain spectroscopy, and second harmonic generation. Integration of surface spectroscopies with electrochemical kinetic techniques under high-temperature/high-pressure aqueous conditions leading to an improved basic understanding of the major factors involved in aqueous corrosion at elevated temperatures. Theoretical (ab initio and molecular dynamics) studies of corrosion-related charge transfer processes supported by parallel electrochemical measurements.

ARGONNE NATIONAL LABORATORY (continued)

061. PARTICLE-SURFACE INTERACTION CHEMISTRY AND CATALYSIS

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

$883,000 03-3

Surface analysis by resonance ionization of sputtered atoms (SARISA) using pico-coulomb ion fluences combined with time-of-flight detection techniques. Development of surface and bulk analytical techniques at the part per trillion level using multiphoton ionization of laser and ion beam desorbed materials. Design and testing of advanced time and energy refocusing high transmission, low noise time-of-flight mass spectrometers. Strong metal-support interactions. Photon-induced desorption cross sections. Adsorbate structures, velocity, and excited state distributions of sputtered species. Mechanism of radiation-enhanced surface segregation in dilute alloy systems. Ion scattering spectroscopy. Correlation of kinetic energies of primary backscattered particles with recoil sputtered surface atoms. Depth of origin of sputtered atoms.

BROOKHAVEN NATIONAL LABORATORY
Upton, NY 11973

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

Metallurgy and Ceramics - 01 -

A. N. Goland - Phone (FTS) 666-3819 or (516) 282-3819
M. Suenaga - Phone (FTS) 666-3518 or (516) 282-3518

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

D. O. Welch, S. M. Heald, J. Tafto, M.W. Ruckman,
S. Usmar, K. G. Lynn, M. Strongin
Phone: (FTS) 666-3517 or 516-282-3517
$482,000 01-1

Experimental and theoretical studies of the fundamental factors which influence the adherence, integrity, stability, and other properties of surface layers of materials which have been modified by various means to have properties different from those within the bulk of the material, e.g., the interface between a coating and a substrate and grain boundaries in intermetallic compounds such as Ni_3Al. Research emphasizes microstructural and chemical characterization and the relation of these characteristics to physical and metallurgical properties using techniques such as glancing angle X-ray reflection and absorption, photoemission, positron annihilation, and transmission electron microscopy.

071. MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS

H. S. Isaacs, K. Sieradzki, J. S. Kim
Phone: (FTS) 666-4516 or (516) 282-4516
$429,000 01-2

Experimental studies of brittle fracture of ductile metals and alloys during stress-corrosion cracking, role of thin surface films, correlation of acoustic and electrochemical noise during cracking with crack arrest marks, intergranular stress-corrosion cracking of Fe-P alloys. Molecular dynamic and analytic modeling of environmentally induced fracture processes. Modeling and experimental studies of initiation of localized corrosion and electrical and structural properties of passive oxide layers, measurement of the electrochemistry within localized sites using a scanning vibrating probe to determine current distributions.

BROOKHAVEN NATIONAL LABORATORY (continued)

072. SUPERCONDUCTING MATERIALS

D. O. Welch, M. Suenaga, J. Tafto, N. Sadakata
Phone: (FTS) 666-3517 or (516) 282-3517
$604,000 01-3

Fundamental properties of high critical temperature and critical field superconductors, effects of strain, disorder, and lattice defects on superconducting properties, theoretical models of interatomic forces, lattice defects, and diffusion kinetics in A15 compounds, annealing and layer growth kinetics in A15 compounds, studies by electron microscopy of lattice defects in superconducting compounds, flux pinning, properties of composite superconductors, new methods of fabricating superconducting materials.

073. PHYSICAL PROPERTIES OF METAL-INTERSTITIAL SYSTEMS

M. S. Pick, S. M. Heald, D. O. Welch
Phone: (FTS) 666-3517 or (516) 282-3517
$491,000 01-3

Studies of physical and metallurgical factors which influence the behavior of interstitial solutes in metals and alloys, studies of the role of microstructure, lattice defects, alloying effects, and surface properties on the thermodynamics, kinetics, and mechanisms of hydrogen uptake and release in transition metals, solid solutions, and intermetallic compounds, effect of dissolved hydrogen upon fracture strength, structural and microstructural studies of metal-interstitial systems using optical, neutron, and X-ray diffraction, EXAFS, electron microscopic, nuclear depth profiling, and surface sensitive techniques, statistical mechanics of metal-interstitial systems.

BROOKHAVEN NATIONAL LABORATORY (continued)

Department of Chemistry - 02 -

A. P. Wolf - Phone (FTS) 666-4397 or (516) 282-4376

074. NEUTRON SCATTERING

J. M. Hastings, R. Thomas
Phone: (FTS)-666-4377 or (516) 282-4377
$433,000 02-1

Neutron scattering studies of the statistical mechanics of phase transitions, the dynamical properties and configurations of magnetic materials, and also crystal structures where relevant. The measurement of the spatial distribution of magnetization and the behavior of spontaneous fluctuations, both of which are essential to understanding magnetic phase diagrams and associated first- and second-order transitions. Because of the universal nature of critical phenomena, information gained from magnetic systems benefit studies of other systems exhibiting second-order phase transformations, such as simple and multicomponent liquids, alloy systems, and superfluids.

Solid State Physics - 02 -

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

075. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

S. M. Shapiro, M. E. Chen, H. Graf, H. Grimm, J. Martinez,
Y. J. Uemura, H. Yoshizawa
Phone: (FTS) 666-3822 or (516) 282-3822
$1,180,000 02-1

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

BROOKHAVEN NATIONAL LABORATORY (continued)

076. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES

G. Shirane, P. Boni, A. I. Goldman, Y. Ito, J. Z. Larese,
C. F. Majkrzak, L. Passell
Phone: (FTS) 666-3732 or (516) 282-3732
$1,450,000 02-1

The principal objective of this program is the investigation of the structure and dynamics of ordered and partially ordered condensed matter using elastic and inelastic neutron spectroscopy. The program has two other objectives as well: (i) the development and evaluation of new techniques for neutron scattering measurement and (ii) the replacement of certain existing High Flux Beam Reactor (HFBR) instruments with new instruments of improved capability. In regard to the latter category, a polarized neutron, triple-axis spectrometer has been completed as part of a joint US-Japan collaborative program and priority is now being given to the development of a time-of-flight mode of operation. Conceptual designs for a neutron spin echo spectrometer and a powder diffractometer have been completed and simple prototypes are now being designed and tested.

077. EXPERIMENTAL RESEARCH - X-RAY SCATTERING

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

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

BROOKHAVEN NATIONAL LABORATORY (continued)

078. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

K. G. Lynn, Y. C. Chen. R. Mayer, J. Throwe
Phone: (FTS) 666-3710 or (516) 282-3710
$945,000 02-2

Investigations of perfect and imperfect solids, interfaces and their surfaces by newly developed experimental methods using variable energy positron and positronium beams coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron Diffraction, Thermal Desorption Spectroscopy). These tools include two-dimensional angular correlation of annihilation radiation, positronium scattering, surface state lifetimes, positron diffusion lengths, positron work functions, positronium formation with measurement of its emitted energy distribution on surfaces, metal-metal and metal-semiconductor interfaces, ion implanted and strain layer superlattices.

079. STRUCTURAL CHARACTERIZATION OF MATERIALS USING POWDER DIFFRACTION TECHNIQUES

D. E. Cox, K. G. Lynn, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516) 282-3818/3870
$325,000 02-2

Utilization of synchrotron radiation for high resolution powder diffractometry and for energy-dispersive diffraction studies of materials at high pressures. Development and application of profile methods for structural analysis of neutron and X-ray powder diffraction data. Orientation of crystals. Preparation of Ni and NI_3Al + B metal films as samples for structural investigations and possible use as positron moderators. Preparation and characterization of bulk inorganic materials.

080. THEORETICAL RESEARCH

P. Bak, J. Davenport, G. J. Dienes, V. J. Emery, K. A. Muttalib, R.M. Sternheimer, G. Vineyard, R. E. Watson, M. Weinert, K. Wiesenfeld
Phone: (FTS) 666-3798 or (516) 282-3798
$840,000 02-3

Phase transitions, critical and cooperative phenomena in magnetic systems, organic metals and incommensurate structures, properties of one- and two-dimensional materials by analytical and numerical methods, nonlinear systems, metal surfaces and adsorbed films, surface states, electronic structure of metals and alloys, X-ray and neutron scattering, photoemission and inverse photoemission, properties of disordered materials and crystal defect physics, high pressure, high temperature properties of solids.

BROOKHAVEN NATIONAL LABORATORY (continued)

081. SURFACE PHYSICS RESEARCH

M. Strongin, S. L. Qui, P. D. Johnson, S. Hulbert, M. L. Shek
Phone: (FTS) 666-3763 or (516) 282-3763
$865,000 02-5

Synchrotron Radiation as a technique to study the geometrical and electronic properties of surfaces and interfaces. The use of new spectroscopies such as inverse photoemission, and the construction of an undulator beam line at the NSLS to enable spin polarized photoemission experiments for studies of the magnetic properties of surfaces. Support has also been given to the development of low-temperature techniques which can be used at the NSLS. The problems presently being studied include: a) electronic properties of overlayers, clean metal surfaces and interfaces; valence band photoemission, inverse photoemission and core level spectroscopy are used as tools in this area, b) organic molecules on surfaces and properties of organic solids, c) surface metallurgy and surface compounds, d) cooperative effects and phase transitions in adsorbate layers on metal surfaces, e) studies of metal clusters in rare gases and in organic solids, f) studies of oxidation and other chemical reactions at low temperatures.

High Flux Beam Reactor - 02 -

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

082. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS

M. H. Brooks, D. C. Rorer, R. C. Karol, L. Junker, D. G. Pitcher, O. Jacobi, S. Protter, R. Reyer, P. Tichler, J. Detweiler, W. Brynda
Phone: (FTS) 666-4061 or (516) 282-4061
$9,976,000 02-1

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

BROOKHAVEN NATIONAL LABORATORY (continued)

National Synchrotron Light Source -02-

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

083. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT

M. Knotek, M. Barton, K. Batchelor, R. Blumberg, J. Galayda, J. Godel, J. Hastings, R. Heese, H. Hsieh, R. Klaffky, S. Krinsky, A. Luccio, C. Pellegrini, W. Thomlinson, B. Craft, A. Van Steenbergen, G. Vignola, J. M. Wang, G. Williams
Phone: (FTS) 666-4966 or (516) 282-4966
$10,811,000 02-2

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

BROOKHAVEN NATIONAL LABORATORY (continued)

Engineering Chemistry - 03 -

A. N. Goland - Phone (FTS) 666-3819 or 516-282-3819
M. Suenaga - Phone (FTS) 666-3518 or 516-282-3518

084. SYNTHESIS AND STRUCTURES OF NEW CONDUCTING POLYMERS

T. A. Skotheim, Y. Okamoto, C. Yang
Phone: (FTS) 666-4490 or (516) 282-4490
$195,000 03-2

Development of a fundamental understanding of ionically and electronically conducting polymers. Research consists of the synthesis of new conducting polymers, the exploration of their physical properties, and the structural characterization by X-ray and neutron diffraction, electron microscopy, magnetic susceptibility, and electrical resistivity measurements. Also included are theoretical studies of the electronic structure and phase transitions of low-dimensional solids and the charge-transfer properties of new conducting polymers. The materials of interest are linear polyethers, polypyrrole, polysilane, etc. This is a collaborative program between Brookhaven National Laboratory and the Polytechnic Institute of New York.

IDAHO NATIONAL ENGINEERING LABORATORY
550 2nd Street
Idaho Falls, ID 83401

V. Storhok - Phone (FTS) 583-8135 or (208) 526-8135

Materials Processing Branch - 01 -

J. F. Key - Phone (FTS) 583-8332 or (208) 526-8332

100. MATERIALS SCIENCE WELDING RESEARCH

J. F. Key, S. A. Chavez, H. G. Kraus
Phone: (FTS) 583-8332 or (208) 526-8332

$190,000 01-5

Establishment of quantitative relationships between materials and processes used to weld them. Emphasis on predicting structure and properties of a weldment from process parameters and materials chemistry. Solidification and microstructure/properties correlations utilizing infrared thermography, moire interferometry high-speed X-radiography, optical and electron microscopy, calorimetry, and computer modeling. Technology transfer through American Welding Institute.

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

C. P. Flynn - Phone (217) 333-1370

Metallurgy and Ceramics - 01 -

H. K. Birnbaum - Phone (217) 333-4778 or (217) 333-1901

105. EFFECT OF TRANSPORT PROCESSES ON LOCALIZED CORROSION

R. C. Alkire
Phone: (217) 333-3640
$70,000 01-1

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

106. CENTER FOR MICROANALYSIS OF MATERIALS

J. A. Eades, C. Loxton, J. Woodhouse
Phone: (217) 333-8396, (217) 333-0386, or (217) 333-3888
$260,000 01-1

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

107. RAPID SOLIDIFICATION PROCESSING

H. L. Fraser
Phone: (217) 333-1975
$160,000 01-1

Development of rapid solidification processing of alloys with powder preparation by laser, spin and centrifugal atomization and subsequent consolidation by dynamic compaction techniques. Characterization of microstructure and measurement of properties developed by heat treatments. Understanding structure-property relationships, mechanisms of metastable phase formation and transformations.

UNIVERSITY OF ILLINOIS MRL (continued)

108. SEMICONDUCTOR CRYSTAL GROWTH BY ION-BEAM SPUTTERING

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

$130,000 01-1

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

109. PROCESSING AND CHARACTERIZATION OF NOVEL AMORPHOUS MATERIALS AND SURFACES

J. M. Rigsbee
Phone: (217) 333-6584

$30,000 01-1

Laser processing to modify structure, composition and physical properties of metallic and ceramic surfaces. Erosion and abrasion resistant surfaces. Physical vapor deposition studies of metastable $Cu_xCr_{(1-x)}$ alloys.

110. MICROCHEMISTRY OF SOLIDS

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

$65,000 01-1

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

111. PROCESSING AND MICROSTRUCTURE OF COMPLEX CERAMIC SYSTEMS

A. Zangvil
Phone: (217) 333-6829

$100,000 01-1

Microstructure and microchemistry of SiC with covalent additives, such as AlN, BN and BeO; solid solution formation in SiC based systems; effect of processing variables and additives on polytypism and microchemistry. Interfaces and toughening mechanisms in SiC- and mullite-matrix composites.

UNIVERSITY OF ILLINOIS MRL (continued)

112. HYDROGEN BEHAVIOR IN BCC METALS

H. K. Birnbaum
Phone: (217) 333-1901

$75,000 01-2

Mobility of hydrogen and deuterium in bcc. metals such as niobium. Gorsky Effect, stress induced reorientation, piezoresistance, acoustic techniques used to study low temperature mobility and interaction of hydrogen with trapping sites. Behavior of hydrogen at surfaces and transfer of hydrogen across surfaces. Phase transitions in the high concentration metal-hydrogen alloys studied with X-rays, neutrons, and acoustic techniques.

113. MICROMECHANICS AND MICROMECHANISMS OF FRACTURE

H. K. Birnbaum, C. J. Alstetter, F. A. Leckie, R. M. McMeeking, D. Socie, J. F. Stubbins, I. Robertson
Phone: (217) 333-1901

$475,000 01-2

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

114. COUNCIL ON MATERIALS SCIENCE

C. P. Flynn
Phone: (217) 333-1370

$85,000 01-2

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

UNIVERSITY OF ILLINOIS MRL (continued)

115. PHYSICAL PROPERTIES OF CERAMIC MATERIALS

W. S. Williams
Phone: (217) 333-3524

$55,000 01-2

Synthesis of low-friction, corrosion-resistant thin films of amorphous carbides and borides by organometallic CVD, thermal vaporization and sputtering. Analysis of film chemistry by XPS, SIMS and AES. Use of EXAFS, EXELFS and computer modeling to obtain radial distributions. Yield behavior of deformation-resistantsingle-phase materials, at high temperature.

116. STRUCTURE AND PROPERTIES OF SILICATE GLASSES AND SILICIDE THIN FILMS

H. Chen
Phone: (217) 333-7636

$75,000 01-3

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

117. A MOLECULAR BUILDING-BLOCK APPROACH TO THE SYNTHESIS OF CERAMIC MATERIALS

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

$100,000 01-3

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

UNIVERSITY OF ILLINOIS MRL (continued)

118. DIELECTRIC SOLIDS

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

$120,000 01-3

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

119. MICROSTRUCTURE AND CRYSTALLIZATION IN NOVEL GLASSY SYSTEMS

S. H. Risbud
Phone: (217) 333-2885

$20,000 01-3

Glass synthesis and phase transformations in quasi-binary II-IV-V_2 semiconducting glasses. Electrical, optical and thermomechanical properties of these glasses. Melting, solidification, and glass formation in quasi-binary systems of the Cd-Zn-Ge-As system. Location of N in crystallized glasses. Formation of glass-ceramic composites.

120. MICROWAVE STUDIES OF TUNNELING STATES IN DISORDERED MATERIALS

H. J. Stapleton
Phone: (217) 333-0037

$60,000 01-3

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

121. PROCESSING OF MONODISPERSE CERAMIC POWDERS

C. Zukoski
Phone: (217)-333-7379

$65,000 01-3

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

UNIVERSITY OF ILLINOIS MRL (continued)

122. RADIATION DAMAGE IN METALS AND SEMICONDUCTORS

I. M. Robertson
Phone: (217) 333-6776

$95,000 01-4

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

Solid State Physics - 02 -

C. P. Flynn - Phone (217) 333-1370

123. LOW-TEMPERATURE STUDIES OF DEFECTS IN SOLIDS

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

$95,000 02-2

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

124. ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES

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

$145,000 02-2

Synchrotron radiation photoemission studies of electronic properties and growth behaviors of semiconductor surfaces and interfaces prepared in-situ by molecular beam epitaxy; properties and atomic structure of alloy surfaces.

125. HIGH-FIELD SUPERCONDUCTORS

D. M. Ginsberg
Phone: (217) 333-4356

$50,000 02-2

Investigation of high-field superconductors by preparation and detailed characterization of samples and by measurements of critical magnetic field, specific heat, magnetic susceptibility, and neutron diffraction.

UNIVERSITY OF ILLINOIS MRL (continued)

126. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER

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

$70,000 02-2

Investigation by ultrasonic methods of impurity--self interstitial interactions in electron irradiated metals and semiconductors, and of hydrogen in bcc metals.

127. INVESTIGATIONS OF CRYSTAL GROWTH BY MOLECULAR BEAM EPITAXY

H. Morkoc
Phone: (217) 333-0722

$200,000 02-2

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

128. PROPERTIES OF CRYSTALLINE CONDENSED GASES

R. O. Simmons, V. R. Pandharipande
Phone: (217) 333-4170 or (217) 333-8079

$190,000 02-2

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

129. NUCLEAR MAGNETIC RESONANCE IN SOLIDS

C. P. Slichter
Phone: (217) 333-3834

$190,000 02-2

Investigations of layered materials and one dimensional conductors with charge density waves, of Group VIII metal-alumina catalysts, and of spin glasses using nuclear magnetic resonance methods.

UNIVERSITY OF ILLINOIS MRL (continued)

130. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS

H. Zabel
Phone: (217) 333-2514

$145,000 02-2

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

131. THE USE OF VERY HIGH PRESSURE TO INVESTIGATE THE ELECTRONIC STRUCTURE OF MATTER

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

$210,000 03-1

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

132. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS

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

$70,000 03-1

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

LAWRENCE BERKELEY LABORATORY
1 Cyclotron Road
Berkeley, CA 94720

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

Materials and Molecular Research Division - 01 -

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

140. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES

R. Gronsky
Phone: (FTS) 451-5674 or (415) 486-5674
$189,000 01-1

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

141. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS

G. Thomas
Phone: (FTS) 451-5656 or (415) 486-5656
$540,000 01-1

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

142. SOLID-STATE PHASE TRANSFORMATION MECHANISMS

K. H. Westmacott
Phone: (FTS) 451-5663 or (415) 486-5663
$189,000 01-1

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

LAWRENCE BERKELEY LABORATORY (continued)

143. NATIONAL CENTER FOR ELECTRON MICROSCOPY

G. Thomas
Phone: (FTS) 451-5656 or (415) 486-5656
R. Gronsky
Phone: (FTS) 451-5674 or (415) 486-5674
K. H. Westmacott
Phone: (FTS) 451-5663 or (415) 486-5663

$1,330,000 01-1

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

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

J. W. Evans
Phone: (415) 642-3807

$70,000 01-1

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

145. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS

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

$136,000 01-1

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

LAWRENCE BERKELEY LABORATORY (continued)

146. COLLABORATIVE RESEARCH BY TRANSMISSION ELECTRON MICROSCOPY

N. E. Phillips
Phone: (FTS) 451-6062 or (415) 486-6062
$48,000 01-1

To foster collaborative research between scientists with specialized skills in advanced techniques of transmission electron microscopy and scientists from other disciplines with projects requiring sophisticated microstructural characterization. Postdoctoral or more mature visiting electron microscopists spend up to one year at LBL using the instrumentation available at the National Center for Electron Microscopy (NCEM) in collaborative programs in the Materials and Molecular Research Division Investigators recommended for support by the NCEM Steering Committee.

147. MECHANICAL PROPERTIES OF CERAMICS

A. G. Evans
Phone: (415) 642-7347
$231,000 01-2

Mechanical reliability of ceramics at high temperatures. The development of predictive capabilities for the high-temperature failure of ceramics and for defect development during sintering. Elevated-temperature failure studies concerned with the initiation, growth, and coalescence of cracks during creep. Experimental measurements are correlated with theoretical models containing the dominant microstructural variables. Sintering studies examining the processes that dictate the development of stresses and defects during solid-state and liquid-phase sintering.

148. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS

R. O. Ritchie
Phone: (FTS) 451-5798 or (415) 486-5798
$274,000 01-2

To examine, from both macroscopic and microscopic perspectives, the mechanics and micro-mechanisms of the sub-critical and critical growth of cracks in engineering materials. Current emphasis is devoted a) to the statistical modeling of crack initiation and crack growth toughness for fracture in low strength steels by cleavage and void coalescence, b) to defining the role of crack tip shielding in influencing the initiation and growth of long and short cracks, particularly for fatigue in dual-phase microstructures, and c) to identifying mechanisms of transient fatigue crack growth during variable amplitude loading in titanium alloys. The aim of the work is to develop a mechanistic understanding of fracture processes in order to provide guidelines for improved life prediction and the alloy design of superior fracture-critical materials.

LAWRENCE BERKELEY LABORATORY (continued)

149. HIGH-TEMPERATURE REACTIONS

A. W. Searcy
Phone: (FTS) 451-5900 or (415) 486-5900
$293,000 01-3

Sintering studies with ultrafine particles of crystalline 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.

150. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS

J. Washburn
Phone: (FTS) 451-6254 or (415) 486-6254
$293,000 01-3

Semiconductor/metal and semiconductor/insulator interfaces with particular emphasis on ohmic and rectifying contacts to GaAs and other 3-5 compounds. Identification of interface phase formation. Study of factors affecting lateral uniformity and correlation with electrical behavior. High resolution transmission electron microscopy and microanalytical techniques are combined with complementary observations on the same specimens such as electron paramagnetic resonance, secondary ion mass spectroscopy, X-ray diffraction and optical or electrical measurements.

151. CHEMICAL PROPERTIES AND PROCESSING OF ADVANCED STRUCTURAL CERAMICS

L. C. De Jonghe
Phone: (FTS) 451-6138 or (415) 486-6138
$440,000 01-3

Structure and chemical stability of Ni/ZrO2 interfaces; behavior of interfaces in thermal barrier coatings. Fundamentals of densification of homogeneous and heterogeneous powder compacts. Simultaneous study of creep and densification using loading dilatometry. Surface chemistry characterization and manipulation, and densification of silicon carbide and silicon nitride powders. Polymer/powder methods. Densification of particulate composites. Sol-gel powders. Use of electron microscope methods, photoelectron spectroscopy, Auger analysis, infrared spectroscopy.

152. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS

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

$91,000 01-3

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

153. CERAMIC INTERFACES

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

$123,000 01-3

Development of an improved understanding of processes that dictate microstructural changes occurring during both materials fabrication and utilization. Current efforts directed at: development of thermodynamic and kinetic descriptions of the stability of continuous intergranular phases, theoretical assessment of the effects of anisotropic surface and grain-boundary energies on microstructural evolution during sintering, modeling the effects of concurrent grain-boundary migration and tracer self diffusion on calculated apparent grain-boundary diffusivities, and examination of the effects of crystallization and sintering atmosphere on microstructure evolution in compacts of chemically synthesized, amorphous, "monodispersed" TiO_2.

154. FAR-INFRARED SPECTROSCOPY

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

$203,000 02-2

Improved infrared detectors, mixers, and spectrometers are developed and used in experiments in important areas of fundamental and applied physics. Technological developments include a liquid-helium-cooled grating spectrometer for emission spectroscopy, ultrasensitive photoconductive detectors for the 50-200 m 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.

LAWRENCE BERKELEY LABORATORY (continued)

155. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS

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

$241,000 02-2

Emphasis on development of linear and nonlinear optical methods for material studies and applications of these methods to probe properties of gases, liquids, and solids. Both theoretical and experimental investigation of various aspects of laser interaction with matter. Development of new nonlinear optical techniques to study isotope separation, photochemistry, molecular clusters, phase transitions, surfaces and interfaces.

156. EXCITATIONS IN SOLIDS

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

$165,000 02-2

Studies of nonlinear dynamics and instabilities in solid state systems. The objectives are detailed experimental studies of driven plasma instabilities in semiconductors; spin wave instabilities in magnetic materials; semiconductor junctions; and ferroelectric materials. These display period-doubling bifurcations, quasiperiodic behavior, mode locking, and onset of aperiodic noise-like behavior, controlled by a fractal attractor. The observed behavior is compared to computed behavior from various theoretical models. The project is a basic science effort with emphasis on a universal understanding of nonlinear dynamics. The results bear directly on the technology of plasmas, solid state devices, and magnetic materials.

157. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS

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

$113,000 02-2

The main objective of this project is to utilize picosecond and subpicosecond laser sources to study the ultrafast relaxation processes that occur in laser-induced annealing and melting. Such processes under investigation include electron-phonon interactions, phonon-phonon interactions, and electron-electron interactions. The experiments involve exciting dense electron-hole plasmas in a semiconductor 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 nonradiative recombinations of photoexcited carriers at deep traps in semiconductors introduced by doping or electron and neutron irradiation. In addition, nonequilibrium phonons generated during the recombination are monitored by Raman scattering.

LAWRENCE BERKELEY LABORATORY (continued)

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

J. Clarke
Phone: (415) 642-3069

$241,000 02-2

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

Accelerator and Fusion Research Division - 02 -

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

159. R&D FOR ADVANCED PHOTON SYSTEMS

M. R. Howells, D. T. Attwood, M. Cornacchia, J. N. Marx
Phone: (FTS) 451-4949

$847,000 02-2

The synchrotron radiation community is now on the threshold of developing a new generation of X-ray facilities that will produce radiation which is extremely bright, powerful, and in some cases partially coherent. In the past, this program has addressed design studies of next-generation undulators and the design and fabrication of high-thermal-loading beamline hardware. During FY86 work entailed preconstruction R&D for a 1- to 2-GeV synchrotron radiation source. Activities include accelerator physics studies, vacuum system studies, instrumentation studies, rf system studies, and impedance studies.

LAWRENCE BERKELEY LABORATORY (continued)

160. CENTER FOR X-RAY OPTICS

D. Attwood
Phone: (FTS) 451-4463 or (415) 486-4463
$1,135,000 02-2

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

161. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES

L. M. Falicov
Phone: 415-642-5993
$70,000 02-3

The purpose of this program is to study properties of solid surfaces. In particular the interest is in determining: (A) structural properties of surfaces, namely the organization and arrangement of atomic constituents at equilibrium, (B) constitutional properties of the surface, in particular the segregation properties of alloys at the surface as a function of crystal structure, surface orientation, nominal chemical composition, and temperatures, (C) electronic structure of surfaces, in particular electron states and electron densities in the neighborhood of the surface, (D) vibronic properties of surfaces, (E) magnetic properties of surfaces, both in magnetic solids (ferromagnetic and antiferromagnetic) and in nonmagnetic solids that may develop a magnetic surface layer, (F) chemical--in particular the catalytic--properties of solids as they are related to basic physical properties (A)-(E).

LAWRENCE BERKELEY LABORATORY (continued)

162. THEORETICAL SOLID-STATE PHYSICS

M. L. Cohen
Phone: (415) 642-4753

$99,000 02-3

Use of microscopic theory based on quantum mechanics to explain and predict properties of real materials. Application to semiconductors, metals, insulators, semimetals, clusters of atoms, and molecules. Emphasis on electronic, vibrational, optical, superconducting, and structural properties of bulk solids. Surfaces and interfaces modeled using microscopic theory.

163. SURFACE, CHEMISORPTION, AND THEORY OF SOLIDS

S. G. Louie
Phone: (415) 642-1709

$57,000 02-3

To further basic understanding of the physical properties of materials and materials systems such as surfaces and interfaces. Emphasis on quantum-mechanical calculations to obtain a microscopic understanding from first principles. Studies include bulk materials, surfaces and chemisorption systems, interfaces, and defects in solids. Bulk materials research is focused on: electronic, structural, and vibrational properties, crystal structure determination, solid-solid phase transformations, and defects properties. Surface and interface research focused on: atomic and electronic structures, mechanisms for structural relaxations and reconstruction, and energetics of adsorbed species.

164. LOW-TEMPERATURE PROPERTIES OF MATERIALS

N. E. Phillips
Phone: (FTS) 451-6063, (415) 486-6063, or (415) 642-4855

$100,000 03-1

Understanding the behavior of materials by measurement of their low-temperature properties, particularly specific heats. Much work in the region below 1 K, where the temperature scale is not well established. Research also conducted on methods of temperature measurement. A temperature scale has been developed to 5 mK. Measurements on ^3He in the Fermiliquid region that have established the correct values of important parameters; measurements on potassium, rubidium, and cesium to 0.06 K to test theoretical predictions of charge-density-wave effects; measurements on CuMn in high magnetic fields that have mapped out the phase boundary of the spin-glass phase; and measurements on a number of heavy-fermion compounds, including two of the three heavy-fermion superconductors, UPt_3 and Ube_{13}. Future objectives include an extension of the ^3He measurements to the superfluid phases, studies on spin glasses, and specific-heat measurements at pressures to 20 kbar and in magnetic fields to 9 T on other heavy-fermion compounds.

LAWRENCE BERKELEY LABORATORY (continued)

165. ELECTROCHEMICAL PROCESSES

C. W. Tobias
Phone: (FTS) 451-5208 or (415) 486-5208
$89,000 03-1

Exploration of novel methods for reducing mass transfer resistance in high rate applications, including in electroforming of metals, and in electrosynthesis. The effects of suspended inert solid 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 for the control of composition and of phase structure in the electrodeposition of alloys. New reaction schemes are evaluated for the efficient electrosynthesis of essential chemicals.

166. HIGH-TEMPERATURE THERMODYNAMICS

L. Brewer
Phone: (FTS) 451-5946 or (415) 486-5946
$141,000 03-3

Development of models of predictive capability for the behavior of gases at high temperatures, of refractory containment materials, and of many metallic systems. The main thrust of the present research aimed at providing quantitative predictive models for the strongly interacting alloys exhibiting generalized Lewis Acid-base behavior. A variety of experimental methods used to characterize the thermodynamics of these systems.

167. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES

D. R. Olander
Phone: (415) 642-7055
$241,000 03-3

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

LAWRENCE BERKELEY LABORATORY (continued)

168. ELECTROCHEMICAL PHASE BOUNDARIES

R. H. Muller
Phone: (FTS) 451-6079 or (415) 486-6079
$141,000 03-3

Study of solid-liquid interfaces: Nucleation and growth mechanisms of the electrocrystallization of metals; effect of adsorbed surface-active materials. Electrolytic metal deposition at high rates; influence of mass transfer conditions on the micromorphology of deposits. Enhancement of rate and uniformity of electrochemical mass transfer by use of suspended solid particles; mechanism of the particle-surface interaction. Surface forces responsible for the formation of thin electrolyte films on metals. Development of optical techniques for measurements of surfaces and thin films at solid-liquid interfaces.

169. SOLID-STATE AND SURFACE REACTIONS

G. A. Somorjai
Phone: (415) 642-4053
$331,000 03-3

Studies of catalyzed surface reactions and investigations of the atomic structure of solid surfaces and adsorbed monolayers. The kinetics and mechanisms of catalytic surface reactions studied using well-characterized crystal surfaces at low and high pressures by using a combination of surface science techniques. Focus on platinum, rhodium, iron and its compounds, rhenium, molybdenum, alkali metals and bimetallic alloys. The adsorbates and reactants are mostly hydrocarbons, oxygen, hydrogen and water. Investigation directed toward an atomic scale understanding of the structure and catalytic behavior of metal surfaces, and at developing new catalysts which submastitute for precious metals and exhibit high rates and selectivity.

170. NUCLEAR MAGNETIC RESONANCE

A. Pines
Phone: (FTS) 451-6097 or (415) 486-6097
$556,000 03-3

Research on methods in magnetic resonance spectroscopy and study of molecular behavior in condensed phases. Novel methods developed include multiple quantum spectroscopy high resolution solid state NMR and magic angle spinning, zero field NMR, pulsed laser nuclear double resonance and non-invasive materials imaging. These methods applied to determination of structure and dynamics at the molecular level in a number of materials including ferroelectrics, liquid crystals, polymers, organic crystals and zeolites. New methods of detection developed to increase the sensitivity of detection, in particular using rapidly switched superconducting fields and Josephson junction devices such as SQUIDS.

LAWRENCE BERKELEY LABORATORY (continued)

171. SYNTHESIS OF NOVEL SOLIDS

A. M. Stacy
Phone: (415) 642-3450

$47,000 03-3

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

Center for Advanced Materials - 03 -

J. J. Gilman - Phone (FTS) 451-4755 or (415) 486-4755

172. CAM ELECTRONIC MATERIALS PROGRAM

Eugene Haller
Phone: (415) 486-5294

$835,000 01-3

Basic theoretical and experimental research to: gain understanding and control of the parameters that affect the quality of large-diameter III-V compound semiconductor single crystals and interfaces. Develop and implement novel and advanced characterization techniques. Further the understanding of the large variety of defects and defect interactions on an atomic scale. Effort in bulk crystal growth includes heat-flow and mass-flow modeling for Bridgman furnace. Characterization effort includes atomic resolution microscopy of GaAs lattice, synchrotron radiation studies of dislocations, stacking faults, and precipitates in GaAs wafers, electron paramagnetic resonance spectroscopy to record antisite spectra in neutron-irradiated and pure, semi-insulating material.

LAWRENCE BERKELEY LABORATORY (continued)

173. CERAMIC AND METAL INTERFACES

R. M. Cannon, R. M. Fisher
Phone: (415) 642-9338

$106,000 01-1

The broad purposes are to develop a combined mechanical and microstructural theory of interface adhesion, and to apply it to analyze and to demonstrate means of improving representative technological systems that rely on interfaces between dissimilar materials. Specific objectives are to model the energy for fracture at or near ceramic-metal interfaces, and to develop and apply experimental techniques to determine these energies. Delamination of thin films and stress development within and mechanical degradation of oxide coatings are also being studied within this context, including the effects of novel compositions and improved deposition methods. Advanced characterization techniques assist in relating preparation conditions, composition and post-preparation processing with both interfacial microstructure and bond strength parameters.

174. CAM STRUCTURAL MATERIALS: PROBLEMS IN ALLOY DESIGN

J. W. Morris, Jr.
Phone: (415) 642-3815 or (FTS) 451-6482

$510,000 01-1

Multifaceted program of metallurgical research that is concerned with the science of alloy design. Current research includes work on the following material types: (1) high-strength, high-toughness ferritic steels; (2) carbon steels with exceptional formability; (3) fatigue-resistant Pb-Sn solder contacts; (4) high field superconducting wire. Each of these alloy design efforts is supported by theoretical and experimental research on the relevant structure-property and structure-processing relations.

175. CAM STRUCTURAL MATERIALS: LIGHT ALLOYS

J. W. Morris, Jr., T. Devine, R. O. Ritchie, G. Thomas
Phone: (415) 642-3815

$195,000 01-1

Multi-investigator program concerned with the properties and development of advanced Al-Li alloys. Tasks include theory, characterization, mechanical properties, chemical properties and alloy design. Alloy design objectives include alloys for cryogenic use, formable alloys, and ultralight alloys.

LAWRENCE BERKELEY LABORATORY (continued)

176. CAM ADVANCED INSTRUMENTATION FOR SURFACE SCIENCE PROGRAM

J. Clarke
Phone: (415) 642-3069

$423,000 02-5

Development of scanning tunneling microscope for study of surface reconstruction, location of absorbed atoms and molecules, the structure of as-grown semiconductors, and the effects of laser annealing. Development of theoretical techniques for interpretation of scanning tunneling microscope results and determination of surface structures. Linear and nonlinear optical studies of polymers on organic and metal surfaces and surfactants on metal and metal-oxide surfaces using surface plasmons, total reflection, second- and third-harmonic generation, and Raman spectroscopy. Development of a system for the study of far-infrared absorption by atomic and molecular adsorbates deposited on substrates attached to doped Ge thermometers and mounted in a vacuum can at liquid-helium temperatures.

177. CAM POLYMERS AND POLYMER COMPOSITES PROGRAM

M. M. Denn
Phone: (415) 642-0176

$534,000 03-2

Development of scientific basis for prediction and control of microstructure in processing high-performance polymeric materials. Goal is microstructure control and production of shaped objects with sufficient strength, thermal stability, and chemical resistance to allow their use as lightweight structural elements in a variety of environments. Focus on liquid-crystal polymers, block copolymers, and short-fiber polymer composites and on coprocessing, structure control through polymer-solvent-nonsolvent interaction, and molecular-weight distribution control through polymerization reaction engineering. Techniques include solid-state NMR, X-ray diffraction, rheological characterization, a new laser-speckle method, microscopy, classical lubrication theory, colloidal nucleation theory, and Flory-Huggins theory and the development of new finite-element methods.

LAWRENCE BERKELEY LABORATORY (continued)

178. CAM CATALYSIS PROGRAM

G. A. Somorjai
Phone: (415) 642-4053

$792,000 03-3

Synthesis, characterization, and evaluation of surface materials: catalysts, coatings interface compounds and bio-compatible surfaces. Emphases are on microporous solids, metal-oxide interfaces, plasma deposited layers and anchored organometallic molecules to polymer surfaces in the liquid phase. Techniques and instrumentation developments include solid state NMR, scanning tunnel microscopy, electron and laser spectroscopies. The materials under investigation include transition metal carbides, nitrides, alumina silicates, bimetallic (Re-Rt, Su-Pd) systems, oxide-metal (TiO_2-M, Al_2O_3,-M, SiO_2-M) interfaces and oxide-oxide interfaces (MoO_x-Al_2O_3, V_2O_x-SiO_2). Discovery of new, lower cost catalysts with increased selectivity and resistance to degradation in industrial conditions.

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

T. Sugihara - Phone (FTS) 532-6340 or (415) 422-6340

Metals and Ceramics - 01 -

R. M. Alire - Phone (FTS) 532-6340 or (415) 422-6340

190. RAPID SOLIDIFICATION PROCESSING OF ALLOYS: STRUCTURE, PHASE RELATIONS AND PHASE TRANSFORMATIONS

L. Tanner, L. Jacobson
Phone: (415) 423-2653

$384,000 01-1

Preparation of rapidly quenched alloys based on aluminum with beryllium and lithium by arc-hammer splat, ribbon spinning and electron beam surface melting, characterization of microstructures produced at different solidification rates by optical and electron microscopy, high resolution TEM, and atom probe, determination of alloy response to thermal treatments by differential scanning calorimetry, differential thermal analysis and microstructure characterization, correlation of results with current thermodynamic kinetic models of solidification. Employ rapid solidification as a means of preparing alloys of Fe-Pd, Fe-Pt, Au-Ni, etc. in order to investigate phenomena associated with displacive phase transformations.

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

E. N. Kaufmann
Phone: (415) 423-2640

$212,000 01-1

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

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

192. OPTICAL MATERIALS RESEARCH

L. L. Chase, D. Milam, S. Payne, W. Siekhaus, N. Winter
Phone: (415) 422-6270

$687,000 02-2

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

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

J. Browne - Phone (FTS) 843-1600 or (505) 667-1600

Metallurgy and Ceramics

J. F. Smith - Phone (FTS) 843-8455 or (505) 667-8455

200. IRRADIATION-INDUCED METASTABLE STRUCTURES IN METALS AND CERAMICS

F. W. Clinard Jr., R. J. Livak, D. M. Parkin
Phone: (505) 667-5102
$280,000 01-4

Alpha decay self-damage in zirconolite, thorite, and huttonite analogues made by doping with short half-life actinides. Neutron-induced fission fragment damage of U Fe and neutron cascade damage of NiTi alloy. Role of starting composition and crystal structure. Evolution of the amorphous state, localized and generalized atomic disorder, alpha recoil and fission fragment tracks. Simulation of damage by ion irradiation. Characterization of radiation effects by X-ray and electron diffraction, optical and electron microscopy, EXAFS, dilatometry, calorimetry, and resistivity. Changes in density, microhardness, fracture toughness, and resistance to microcracking. Effect of elevated temperature during self-damage, post-irradiation annealing and recovery.

201. MECHANICAL PROPERTIES

M. G. Stout, U. F. Kocks, P. S. Follansbee, P. L. Martin,
D. J. Srolovitz, R. B. Schwarz
Phone: (505) 667-4665
$847,000 01-5

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes, Bouschinger effects. Characteristics of and mechanisms controlling the large strain deformation of aluminum, nickel, copper, brass, substructural and textural evolution with strain, strain state, and strain rate. Predictions of texture evolution using crystal plasticity and strain-rate sensitivity. Kinetics of plastic flow at room and elevated temperatures. Response of metals to high strain rates, Hopkinson split-pressure bar experiments, dislocation dynamics, threshold stress at 0 K, viscous drag. Dynamics of microstructural evolution, Frenkel-Kontorova model of dislocation cores. Self-consistent model of phonon radiation field of moving dislocations. Model includes edge dislocations, screw dislocations, nucleation of dislocation loops. Synthesis and characterization of amorphous alloys. Study of phase equilibria, transformation kinetics of solid-state amorphizing reactions, mechanical alloying, sintering dynamic compaction. Characterization of atomic structure, thermal stability resistance to oxidation and corrosion, magnetic susceptibility. High temperature response of Al O in tension and torsion. Mixed mode brittle fracture at 1100 C. Microstructural effects on high temperature brittle fracture.

LOS ALAMOS NATIONAL LABORATORY (continued)

202. STRUCTURAL CERAMICS

D. S. Phillips, T. N. Taylor, J. J. Petrovic, P. D. Shalek
Phone: (505) 667-5128
$318,000 01-5

Reactivity and electrophoretic mobility of selected SiC powders and whiskers in aqueous and alcoholic media. Modification of those reactivities by annealing under controlled atmospheres. Correlation of reactivity with UHV surface chemistry and with powder microstructure. Colloidal processing of model SiC (w) - SiO and SiC (w) - graphite composites based on these reactivities. Mechanics of crack-whisker interactions in resulting composite materials.

Physics Division - 02 -

J. F. Smith - Phone (FTS) 843-8455 or (505) 667-8455

203. CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY

J. Eckert
Phone: (505) 667-6069
$1,800,000 02-1

Neutron scattering research in condensed matter using the pulsed spallation neutron source at the Los Alamos Neutron Scattering Center (LANSCE). Studies in most areas of condensed matter, currently metal hydrides, catalysts, liquids, metallic glasses, magnetism, crystal structure, and chemical spectroscopy. LANSCE is a national facility for neutron scattering research in solid-state physics, chemistry, materials science, biology, and polymers with the following time-of-flight spectrometers: single-crystal diffractometer, filter difference spectrometer, 32-m neutron powder diffractometer, high intensity powder diffractometer, constant-Q spectrometer, low-Q diffractometer and, in the near future, chopper spectrometer.

204. MATERIALS UNDER EXTREME CONDITIONS

D. Schiferl, R. LeSar, J. K. Hoffer, R. Heffner
Phone: (505) 667-4129
$241,000 02-2

Studies of solidification, crystal structures, phase transformations, and thermodynamics of simple dielectrics, hydrides, and polymers from low to high temperature in high-pressure diamond anvil cells (DACs) using UV, IR, and Raman spectroscopy and laser-beam, neutron, and X-ray scattering, develop theories of phase transformation, structural behavior, and chemical reaction kinetics, use DACs to prepare and characterize exotic materials, including rare-gas and hydrogen-containing molecules.

LOS ALAMOS NATIONAL LABORATORY (continued)

205. CORRELATED ELECTRONS IN METALS

J. L. Smith, Z. Fisk, J. D. Thompson
Phone: (505) 667-4476

$96,000 02-2

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

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

J. C. Wheatley, G. W. Swift, A. Migliori
Phone: (505) 667-4133

$220,000 02-5

Natural or intrinsically irreversible engines: acoustic engines using liquids and gases, heat pumps and prime movers; liquid propylene heat engine: regenerators, heat exchangers, mechanicals, seals; thermal convection in dilute solutions of ^3He in superfluid ^4He near 1 K: steady and oscillatory, nonlinear dynamics, coherence and chaos; spin-polarized hydrogen isotopes: transport, thermodynamic properties, magneto-sound; superfluid liquid ^3He: ferromagnetism, A-->B phase transition dynamics.

Materials Chemistry - 03 -

J. F. Smith - Phone (FTS) 843-8455 or (505) 667-8455

207. SURFACE SCIENCE OF CERAMICS

T. N. Taylor
Phone: (505) 667-7712

$58,000 03-2

Characterization of majority species on SiC powder surfaces using XPS and LEISS. Correlation of surface chemistry with powder preparation and reactivity. Graphitization of SiC surfaces. Powder surface modification by gas phase reaction, with focus toward improving dispersibility. Comparison of orientationally-averaged powder results with model single crystal experiments. Surface bonding (XPS) and subsurface diffusion (RBS) of selected dopants on SiC, especially the beta-form.

208. CONDUCTING POLYMERS AS SYNMETALS

M. Aldissi, A. R. Bishop, D. K. Campbell, R. Liepins, W. C. Overton
Phone: (505) 667-1326

$356,000 03-2

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

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

A. Zucker - Phone (FTS) 624-4321 or (615) 574-4321

Metallurgy and Ceramics - 01 -

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

215. THEORETICAL STUDIES OF METALS AND ALLOYS

W. H. Butler, J. S. Faulkner, G. S. Painter, G. M. Stocks,
D. M. Nicholson
Phone: (615) 574-4845
$685,000 01-1

Use of density functional theory to calculate the properties of materials. Use of KKR-CPA to calculate such properties of alloys as phase diagrams, thermodynamic properties, magnetic properties, lattice constants, short-range order parameters, electrical and thermal resistivities. Use of high-speed band theory (QKKR) to calculate total energies of metals and intermetallic compounds. 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.

216. X-RAY RESEARCH USING SYNCHROTRON RADIATION

C. J. Sparks Jr., G. E. Ice, O. B. Cavin
Phone: (615) 574-6996 ORNL, (516) 282-5614 NSLS
$560,000 01-1

Use of synchrotron radiation as a probe for the study of metal alloy and ceramic systems. Emphasis on the ability to select a particular X-ray energy from the synchrotron radiation spectrum to selectively highlight specific elements. Thus, the atomic arrangements among the various elements forming the materials can be unraveled and related to the materials' physical and chemical properties. Construction and installation of an X-ray beam line on the National Synchrotron Light Source at Brookhaven National Laboratory. Important materials' problems to be considered include: (1) effects of short-range order among atoms on radiation induced swelling and mechanical behavior, (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, rapid cooling, and atomic displacements.

OAK RIDGE NATIONAL LABORATORY (continued)

217. MICROSCOPY AND MICROANALYSIS

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

$705,000 01-1

Development and application of analytical electron microscopy (AEM) and atom-probe field-ion microscopy (APFIM) to determine the microstructure and microchemistry of materials. Equilibrium and radiation-induced segregation at grain boundaries and interfaces by APFIM/AEM, correlation of GB structure and segregation. Characterization of ordered and modulated alloys by direct measurement of diffracted electron intensities. Standardless EELS analysis, cross-section measurements for E_0 < 300 kV. Secondary fluorescence in EDS. Lattice site location in alloys by electron channeling microanalysis. APFIM characterization of modulated structures, spinodals, and early stages of phase transformations. GB phases and segregation in structural ceramics, ion-implanted ceramics, crept SiC, precipitates, segregation, and dislocations in Ni_3Al, AEM of supported metal catalysts.

218. RADIATION EFFECTS

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

$1,385,000 01-4

Mechanisms and theory of radiation effects, neutron damage in pure metals, alloys, and ceramics irradiated in ORR, HFIR, EBR-II and FFTF. Effect of alloying additions; impurities and microstructure on dimensional instability and embrittlement; phase stability under irradiation; radiation effects studies using multiple ion beams (heavy and dual light ions); relationship between ion and neutron damage; effect of helium and other gases on microstructure and microcomposition; theory of void swelling and irradiation creep; solute-defect interactions; cascade diffusion theory, Fe, Al, Zr, Ni, and austenitic Fe-Cr-Ni alloys; ferritic alloys; MgO, Al_2O_3, $MgAl_2O_4$. Ion beam modification of phase relationships, surface-sensitive mechanical properties and microstructure of alloys using multiple simultaneous beams of various species; new materials by ion beam processing.

OAK RIDGE NATIONAL LABORATORY (continued)

219. HIGH TEMPERATURE ALLOY DESIGN

C. T. Liu, C. L. White, M. H. Yoo, J. H. Schneibel,
D. M. Kroeger, J. A. Horton, W. C. Oliver, A. DasGupta,
R. K. Williams, D. S. Easton
Phone: (615) 574-4459

$1,245,000 01-5

Design of ordered intermetallic alloys based on Ni_3Al and other aluminides. 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. Experimental work on structure and properties of rapidly solidified materials and thermal and physical properties of aluminides. Establishment of correlation between mechanical properties, microstructural features, and defect structures in aluminides.

220. PROCESSING SCIENCE AND MECHANICAL BEHAVIOR OF CERAMICS

P. F. Becher, P. Angelini, S. Baik, A. Bleier
Phone: (615) 574-5157

$945,000 01-5

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

OAK RIDGE NATIONAL LABORATORY (continued)

221. FUNDAMENTALS OF WELDING AND JOINING

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

$475,000 01-5

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

222. STRUCTURE AND PROPERTIES OF SURFACES AND INTERFACES

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

$675,000 01-5

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

Solid State Division - 02 -

B. R. Appleton - Phone (FTS) 624-6151 or (615) 574-6151

223. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS

R. M. Nicklow, J. W. Cable, H. R. Child, B. D. Gaulin, M. Hagen,
J. B. Hayter, H. A. Mook, R. M. Moon, H. G. Smith, Y. Tsunoda,
N. Wakabayshi
Phone: (615) 574-5240

$815,000 02-1

Inelastic neutron scattering studies of phonons, magnons, and single-particle excitations in condensed matter, elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials, lattice dynamics of I_2, Sm, UBe_{13}, and graphite intercalation compounds, magnetic excitations in spin glasses, USb, paramagnetic Ni, Fe, Gd, Sm, and $KMn(Ni)F_3$, phase transitions in KTN, Ni_3Mn, Cu(Fe), and random-field systems, nuclear spin ordering in Pr, $PrCu_2$, and $Cs_2NaHoCl_6$ momentum distributions in ^3He and ^4He. New research directions will include more emphasis on materials properties under extreme environments of high pressures, high temperatures or ultralow temperatures.

OAK RIDGE NATIONAL LABORATORY (continued)

224. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES

J. W. Cable, H. R. Child, B. D. Gaulin, J. B. Hayter,
H. A. Mook, R. M. Moon, Y. Morii, R. M. Nicklow, H. G. Smith,
S. Spooner, G. D. Wignall
Phone: (615) 574-5233

$656,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors metal hydrides, and defects in single crystals, lattice dynamics of CeD_2, Fe(Cr) alloys, and KCl(CN), magnetic excitations in CeD_2, PrD_2, and $K_2(Co)FeF_4$, phase transitions in metal alloys, $CoCr_2O_4$, ZrO_2, heavy fermion superconductors and reentrant superconductors, SANS from ferrofluids, micelles under shear, polymers and polymer blends, metal alloys, and biological systems, kinetics of first-order phase transitions.

225. SUPPORT FOR NEUTRON USERS' PROGRAM

R. M. Nicklow, J. W. Cable, H. R. Child, B. D. Gaulin,
M. R. Hagen, H. A Mook, R. M. Moon, H. G. Smith
Phone: (615) 574-5240

$780,000 02-1

ORNL neutron scattering facilities are available to outside scientists through Neutron Users' Program, recent investigations include lattice dynamics and magnetic properties of intercalated graphite, NiAl, LiAl, structure and dynamics of spin glasses, random field systems, polarized-beam studies of paramagnetism, heavy fermion superconductors, quasicrystals, amorphous magnetic materials, proton diffusion in biological systems, and collagen periodicity in bones.

226. PHYSICAL PROPERTIES OF SUPERCONDUCTORS

S. T. Sekula, D. K. Christen, J. R. Ellis, J. R. Thompson
Phone: (615) 574-6271

$335,000 02-2

Investigations of flux-line-lattice arrays, flux motion, flux-line defect interactions, anisotropy in refractory metal alloys and compounds with A15 and B1 crystal structures, and formation of metastable superconductors by rapid laser quenching, small-angle neutron scattering by flux-line lattices in equilibrium and nonequilibrium configurations, dc magnetization, ac magnetic permeability, critical-current and normal-state electrical transport, ion damage and implantation in foil and thin-film superconductors, low-temperature fast neutron irradiation, pulsed-laser irradiation at low temperatures.

227. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION

D. H. Lowndes, M. J. Aziz, G. E. Jellison, D. N. Mashburn,
F. A. Modine, S. J. Pennycook, R. D. Westbrook, R. F. Wood
Phone: (615) 574-6306

$935,000 02-2

Picosecond laser spectroscopy, time-resolved reflectivity, transmissivity, and ellipsometric measurements, time-resolved transient electrical conductivity light-assisted chemical vapor deposition of thin films, modulated layered structures, and superlattices, 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 thermophotovoltaic systems, effects of point defects, and impurities on electrical and optical properties of single-crystal and polycrystalline Si, electrical, optical (including infrared and luminescence spectroscopy), transmission electron microscopy, X-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering measurements, dopant concentration profile, deep-level transient spectroscopy, and absolute quantum efficiency measurements.

228. FUNDAMENTAL ASPECTS OF METAL FRACTURE

F. W. Young, S.-J. Chang, C. G. Park
Phone: (615) 574-5501

$360,000 02-2

Experimental and theoretical studies of microscopic fracture phenomena by transmission electron microscopy and continuum fracture mechanics, in situ TEM observations of crack propagation in metals (bcc and fcc), alloys and ceramics, investigation of the geometry of plastic deformation occurring ahead of crack tip, dislocation model of fracture toughness, theories of plastic zones with a dislocation-free zone ahead of wedge or blunted cracks, direct observations of crack propagation in bcc metals at low temperatures, mechanism of ductile vs brittle fracture of bcc metals, dislocation model of fatigue crack propagation, in situ TEM studies of crack propagation in hydrogen environment, crack tip deformation and crack propagation in neutron irradiated metals and alloys.

OAK RIDGE NATIONAL LABORATORY (continued)

229. HIGH TEMPERATURE CERAMIC MATERIALS

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

$740,000 02-2

Physical and chemical properties of refractory materials, electronic ceramics, and solid ionic conductors, transition-metal carbides and nitrides and refractory oxides, physical properties of materials characterized with regard to composition, defect structures, and phase segregation, studies involving charge and mass transport with emphasis on varistor materials, degradation, and high-temperature effects, electrical transport in single-phase and composite electrolytes, role of adsorbed water on enhanced conductivity in $AgCl-Al_2O_3$ composites, techniques include optical and electron spectroscopies and electrical measurements.

230. SOLID-SOLID INTERFACES

J. B. Bates, D. M. Zehner, Y. T. Chu, J. C. Wang
Phone: (615) 574-6280

$300,000 02-2

Charge transport at metal-dielectric and dielectric-dielectric interfaces and the atomic properties related to the ordering and growth of epitaxial overlayers are investigated by experimental and theoretical techniques, effect of micron and submicron structure on charge diffusion and impedance of metal-insulator contacts, low-frequency and optical dielectric properties and excitation of surface modes at solid-solid boundaries, techniques include small-signal ac response and transit signal analysis, infrared attenuated total reflectance, surface enhanced and micro Raman scattering, model calculations and computer simulation, deposition of controlled amounts of submonolayer and monolayer quantities of atoms on well-characterized surfaces using molecular beam epitaxy, investigation of two-dimensional phenomena related to ordering, migration, and layer growth using LEED, examination of the effects of variation of the parameters related both to the deposition source and to the condition of the substrate.

OAK RIDGE NATIONAL LABORATORY (continued)

231. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS

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

$740,000 02-2

Preparation and characterization of advanced materials including the growth of single-crystal research specimens and the development of new crystal growth techniques, arc fusion and flux growth of high-temperature materials (Y_2O_3, MgO, CaO, SrO, WC), Czochralski and float zone growth of ternary Fe-Ni-Cr alloys (i.e., stainless steels), rf induction float zone growth of transition-metal carbide single crystals, growth of perovskite-structure oxides (e.g., $KTaO_3$, $CaTiO_3$, $KTa_{1-x}Nb_xO_3$), float zone and tri-arc growth of A15 compounds (i.e., V_3Si, Ti_3Pt, V_3Ge), growth of refractory metal single crystals such as Ti, Zr, Ir, Nb, Ta, V, and W by means of the electron beam float zone technique, growth of single crystals of semiconducting oxides (i.e., Ca-doped $KTaO_3$), flux growth of single crystals of fast ion conductors (beta-alumina and beta"-alumina), growth of single crystals with controlled geometries and isotopically enriched research specimens, characterization studies of single crystals using Rutherford backscattering, ion channeling, EPR, neutron scattering, thermal analysis, and other techniques.

232. SMALL-ANGLE X-RAY SCATTERING

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

$170,000 02-2

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

OAK RIDGE NATIONAL LABORATORY (continued)

233. THEORY OF CONDENSED MATTER

J. F. Cooke, J. H. Barrett, F. H. Claro, H. L. Davis, W. Ekardt, L. J. Gray, T. Kaplan, S. H. Liu, G. D. Mahan, D. Meltzer, M. E. Mostoller, O. S. Oen, M. Rasolt, M. T. Robinson, B. Sernelius, K. Shung, K. R. Subbaswamy, J. C. Wang, R. F. Wood
Phone: (615) 574-5787

$1,164,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors, lattice vibrations in metals and alloys, lattice dynamics and potential energy calculations of ionic crystals, computer simulation of radiation damage and sputtering, reflection of light atoms from surfaces, surface studies with backscattered ions, development of LEED theory and interpretation of LEED data, surface vibrations and relaxation, theory of angular effects in photoemission, 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. New directions include: quantum Hall effect, neutron scattering at high energies, development and application of SPLEED theory, diffusion and elastic vibrations of fractal systems.

234. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY

B. C. Larson, J. D. Budai, S. Iida, J. D. Lewis, S. M. Ohr, C. G. Park, S. Pennycook, J. Z. Tischler
Phone: (615) 574-5506

$794,000 02-4

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

OAK RIDGE NATIONAL LABORATORY (continued)

235. SYNTHESIS AND PROPERTIES OF ISOTOPIC SOLIDS

L. A. Boatner, M. M. Abraham, J. O. Ramey, B. C. Sales
Phone: (615) 574-5492
$420,000 02-4

The development of new advanced materials through the application of enriched isotopes, control and tailoring of specific materials characteristics by means of both stable and enriched isotopes, synthesis and growth of isotopically enriched materials for use in detailed materials characterization studies using spectroscopic techniques, the application of isotopic solids to investigations of lead-iron phosphate glasses and related glass systems, isotopic substitution techniques applied to studies of polycrystalline ceramics, metal single crystals, and dielectrics, investigations of physical, chemical, and thermal properties of isotopic solids using the techniques of optical absorption, Raman scattering, Mossbauer spectroscopy, electron paramagnetic resonance spectroscopy, Rutherford backscattering, ion implantation, thermal analysis, and ion channeling, the use of isotropic substitution techniques in the resolution of basic research problems, the development of new materials for applications in materials-related technologies through isotopic substitution.

236. OPERATION AND RESEARCH USE OF A LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

H. R. Kerchner, R. R. Coltman Jr., C. E. Klabunde
Phone: (615) 574-6270
$970,000 02-4

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

OAK RIDGE NATIONAL LABORATORY (continued)

237. SURFACE PHYSICS AND CATALYSIS

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

$895,000 02-5

Studies of crystallographic and electronic structure of clean and adsorbate-covered metallic and semiconductor surfaces, combined techniques of low-energy electron diffraction (LEED), photoelectron spectroscopy (PES) using synchrotron radiation, and computer simulations for surface crystallography studies with emphasis on surfaces which either reconstruct or have interplanar spacings different from those of the bulk, LEED, PES, and Auger electron spectroscopy (AES) combined with in situ laser annealing 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 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.

238. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND COLLABORATIVE RESEARCH CENTER

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

$895,000 02-5

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

OAK RIDGE NATIONAL LABORATORY (continued)

239. ION BEAM ANALYSIS AND ION IMPLANTATION

C. W. White, B. R. Appleton, M. J. Aziz, J. H. Barrett,
C. Buchal, R. J. Culbertson, G. C. Farlow, W. O. Hofer,
C. J. McHargue, D. B. Poker, O. E. Schow, J. M. Williams,
S. Withrow
Phone: (615) 574-6295
$960,000 02-5

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

240. ION BEAM DEPOSITION

J. M. Roberto, B. R. Appleton, N. Herborts, T. S. Noggle,
R. A. Zuhr
Phone: (615) 576-0227 $191,000 02-5

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

OAK RIDGE NATIONAL LABORATORY (continued)

241. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION

W. S. Aaron, H. L. Adair, M. Petek, T. C. Quinby
Phone: (615) 574-5916
$330,000 02-5

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

Materials Chemistry - 03 -

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

242. CHEMISTRY OF ADVANCED INORGANIC MATERIALS

E. J. Kelly, C. E. Bamberger, G. M. Begun, G(ilbert) M. Brown,
J. Brynestad, L. Maya, C. E. Vallet
Phone: (FTS) 624-5024 or (615) 574-5024
$1,168,000 03-1

Application of ion implantation and ion beam mixing to the generation and systematic study of surface-modified materials of interest as catalysts, e.g., mixed oxide catalysts on metallic substrates for electrocatalysis of Cl_2 and O_2 evolution; determination of the mechanism of the catalyzed reaction, nature of the catalyst, and its specific mode of operation via electrochemical, Rutherford backscattering, and in situ photoacoustic and photocurrent spectroscopic techniques. SiS-based methodology for the synthesis of high-purity ceramics (alpha-Si_3N_4, SiC, etc.) from relatively impure silicon; synthesis characterization, pyrolysis and photolysis of groups IV-A, V-A, and VI-A transition metal organometallic compounds for the preparation of ceramic powders, fibers, and films; synthesis of transition metal (Ti, Nb, Mo, V, etc.) nitrides and carbonitrides via precursors generated by ammonolytic and metathetical reactions in liquid ammonia; utilization of molten cyanides for the synthesis of BN and TiN ceramics; application of a metal atom reactor to the synthesis of ceramic and ceramic precursor compounds.

OAK RIDGE NATIONAL LABORATORY (continued)

243. STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS

A. H. Narten, B. K. Annis, G(eorge) M. Brown, W. R. Busing,
E. Johnson, D. W. Noid, W. E. Thiessen
Phone: (FTS) 624-4974 or (615) 574-4974
$1,049,000 03-2

Characterization of polymers and composites at the molecular level by neutron and X-ray scattering studies, prediction of conformational, thermodynamic, and dynamics propertes through advanced computing and statistical mechanical techniques, relationship of structure to physical properties, neutron spectroscopy, development of synchrotron radiation facilities, computational methods for dynamic correction of neutron scattering intensities. Materials studied include high-performance crystalline fibers and composites, ionomers, and small-molecule models for polymers.

244. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY-RELATED MATERIALS

T. B. Lindemer, C. M. Simmons, A. L. Sutton
Phone: FTS 624-6850 or (615) 574-6850
$360,000 03-2

Determination and modeling of phase equilibria and other thermochemical data important to energy-related ceramic systems. Emphasis on the measurement and application of such data for the actinide oxides used as nuclear fuels, but the methodology is applicable to any oxide solid solution. Current studies involve nonstoichiometric dioxides in the system of elements U, O, and either Y, Ce, Nd, Gd, or Eu. Experimental data are obtained under conditions generally not previously investigated. Adaptations of chemical-mathematical models from the literature are used to represent the chemical thermodynamic interrelationship of temperature, oxygen chemical potential, and nonstoichiometry. These efforts provide a heretofore unavailable, generalized chemical thermodynamic description of the actinide-lanthanide dioxide solutions. Exploratory work involves application of this methodology to structural ceramic systems.

OAK RIDGE NATIONAL LABORATORY (continued)

245. CHEMICAL ENGINEERING RESEARCH

C. H. Byers, M. T. Harris
Phone: (FTS) 624-4653 or (615) 574-4653
$305,000 03-2

Fundamental laser scattering measurements and theoretical framework for material transport and thermodynamic properties of liquid mixtures at high temperatures and pressures, often in the critical region. Methods development (including optical measurements, dispersion stabilization, and mathematical analysis) for properties measurement of organic mixtures such as those important in critical extraction. Critical region phase equilibrium. Viscosities, diffusivities, and vapor-liquid equilibrium at high pressures and temperatures. Crystallization and growth of monodispersed seed materials, particle size analysis.

OAK RIDGE ASSOCIATED UNIVERSITIES
Oak Ridge, TN 37831

A. Wohlpart - Phone (FTS) 626-3255 or (615) 576-3255

Metallurgy and Ceramics - 01 -

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

255. OAK RIDGE SYNCHROTRON ORGANIZATION FOR ADVANCED RESEARCH

T. A. Habenschuss, C. J. Sparks, R. DeAngelis, S. Moss, R. Young
Phone: (615) 574-6996 or (FTS) 624-6996
$100,000 01-1

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

256. SHARED RESEARCH EQUIPMENT PROGRAM (SHARE)

E. A. Kenik, K. More
Phone: (615) 574-5066 or (FTS) 624-5066
$95,000 01-1

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

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

Metallurgy and Ceramics - 01 -

G. L. McVay - Phone (FTS) 444-7511 or (509) 375-3762

260. HIGH-TEMPERATURE CORROSION AND ELECTROCHEMICAL INTERACTIONS IN CERAMICS

J. L. Bates, C. F. Windisch
Phone: (509) 375-2579

$330,000 01-1

Mechanisms and kinetics of high-temperature reactions for refractory metal oxides with molten silicates, molten salts, and gases. Dissolution of oxides such as $MgAl_2O_4$, Al_2O_3, MgO, and $Y_3Al_5O_{12}$ with Ca-Al-silicate containing Mg and Fe in oxidizing, reducing, and sulfur-containing atmospheres. Electrochemical interaction and decomposition of oxides such as ZrO_2 in molten salts and silicates. Effects of grain boundary chemistry and structure, crystallographic structure and electrical characteristics on dissolution and electrochemical reactions. Mass transport near reaction interfaces and in grain boundaries from elemental distribution using high resolution, quantitative EDX, electron microprobe, STEM coupled with optical microscopy, TEM, SEM, and AES. Direct in-situ observation of reaction interfaces using laser Raman spectroscopy.

261. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

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

$450,000 01-2

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

PACIFIC NORTHWEST LABORATORY (continued)

262. LEACHING OF GLASS AND CERAMICS

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

$380,000 01-3

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

263. RADIATION EFFECTS IN METALS AND CERAMICS

E. P. Simonen, J. L. Brimhall
Phone: (509) 376-3124

$150,000 01-4

Evaluation of radiation damage mechanisms in metals and nonmetals, irradiation of metals using heavy-ion and neutron bombardment and high-voltage electron microscopy, analyses using analytical electron microscopy, positron annihilation, rate theory microstructural modeling, in situ irradiation creep testing, effects of irradiation on recovery, recrystallization, defect microstructures, precipitate microstructures, and hardening in ferritics. Characterization of localized defect states in glasses and nonmetallic crystals by vibrational Raman spectroscopy and optical absorption. Kinetic studies of damage ingrowth and annealing phenomena using X-ray diffraction, electron microscopy, microhardness testing, and bulk swelling determinations. Model development for damage in nonmetals. Project phasing out.

PACIFIC NORTHWEST LABORATORY (continued)

Solid State Physics - 02 -

G. L. McVay - Phone (FTS) 444-7511 or (509) 375-3762

264. THIN FILM OPTICAL MATERIALS

R. A. Craig, G. J. Exarhos, D. M. Friedrich
Phone: (509) 375-2440

$183,000 02-2

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

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

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

Metallurgy and Ceramics - 01 -

R. J. Eagan - Phone (FTS) 844-4069 or (505) 844-4069

275. PHYSICS AND CHEMISTRY OF CERAMICS

T. A. Michalske, A. Hurd, D. Haaland, B. C. Bunker, K. D. Keefer, D. W. Schaefer, C. J. Brinker, P. Ho, R. E. Loehman, C. H. F. Pedan
Phone: (505) 846-3551

$1,153,000 01-2

Multidisciplinary studies to relate molecular structure of ceramics to physical properties. Develop models for environment/strained solid interactions used to interpret fatigue effects; Photon Stimulated Desorption (PSD) of in situ fracture surfaces to determine chemical compounds resulting from stress corrosion fracture, model systems to study strain-enhanced chemistry; FTIR studies of adsorbate reactions used to relate strain enhanced chemistry and stress corrosion fracture. Characterize sol-to-gel and gel-to-glass transitions in the silica system using SAXS, HPLC, 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 solid material from solution chemistry, and model sintering and absorption characteristics of random porous materials. Study sintering of silicon nitride using oxygen free powders, characterize powder preparation processes.

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

276. STRAINED-LAYER SUPERLATTICE MATERIALS SCIENCE

R. M. Biefeld, L. R. Dawson, I. J. Fritz, P. L. Gourley, D. R. Myers, G. C. Osbourn
Phone: (505) 844-4309

$397,000 01-2

Studies of strained-layer superlattices (SLS's), a new class of semiconductor materials with unique and tailorable electronic and structural properties are expected to have a broad range of device applications. Research emphasizes: electronic energy levels and the effects of Brillouin zone folding on optical transition strengths in SLSs, transport properties and quantum oscillations in SLS structures tailored for large mobilities, conditions for growth and doping of new SLS structures, stability of SLS's subjected to high temperature aging, ion implantation damage and annealing, thermal cycling, and hydrostatic pressure.

SANDIA NATIONAL LABORATORIES (continued)

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

277. ION IMPLANTATION AND DEFECTS IN MATERIALS

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

$920,000 01-3

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

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

278. ADVANCED GROWTH TECHNIQUES FOR IMPROVED SEMICONDUCTOR STRUCTURES

S. T. Picraux, A. W. Johnson, J. Y. Tsao, B. Dodson, T. J. Drummond, I. J. Fritz, P. L. Gourley, J. Washburn (U.C. Berkeley Lab)
Phone: (505) 844-7681

$186,000 01-3

Studies of new approaches to epitaxial thin-film growth techniques. Specific techniques to include: 1) ion- and laser-beam-assisted MBE, 2) ion- and laser-beam-assisted CVD, and 3) ion- and laser-beam-assisted plasma deposition. Addition of localized energy alters growth kinetics and allows wider range of nonequilibrium growth conditions. The work to concentrate on layered III-V compounds, Si/Ge layered structures, and hybrid Si/III-V structures. In-vacuum measurement tools to include electron beam probes (Auger, SIMS, etc.). Laser Raman and laser scattering from surface during growth of epitaxial film to be explored as in situ measurement tool. Theoretical investigations of epitaxial growth under nonequilibrium conditions, stability of film under post deposition processing, impurity diffusion in layered structures.

SANDIA NATIONAL LABORATORIES (continued)

Solid State Physics - 02 -

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

279. SURFACE PHYSICS RESEARCH AND STIMULATED DESORPTION

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

$608,000 02-2

The goal of this program is to develop a fundamental understanding of the physics underlying the modification and control of surfaces by studying their electronic and structural properties. The near term emphasis is on exploring the exciting properties of strained-metal overlayers and on issues related to the important technological areas of oxidation, adhesion, and the sintering and fracture of ceramic materials. Strong features of this program are the ability (1) to apply techniques which probe the properties of modified surfaces at the local atomic level, (2) to couple this with theoretical support, and (3) to have direct working relationships with applied programs in a multidisciplinary approach which ensures technological impact. The program encompasses experimental and theoretical efforts in ultra-violet photoemission spectroscopy (UPS), low energy electron loss spectroscopy (LEELS), imaging and pulsed-laser atom-probe mass spectroscopy, field ion microscopy, and Auger lineshape analysis.

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

280. ORGANIC CONDUCTORS AND SUPERCONDUCTORS

L. J. Azevedo, D. S. Ginley, J. F. Kwak, P. F. Nigrey, J. E. Schirber
Phone: (505) 844-8134

$327,000 02-2

The fundamental physical properties of the charge transfer organic superconductors and the polymeric organic conductors. Directed toward understanding the detailed band structure, doping, and carrier transport in these materials, especially as they pertain to understanding metal-insulator transitions, superconductivity, and the role of disorder in determining transport properties. Unique and specialized instrumental capabilities including high frequency magnetic resonance, 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 in collaboration with J. Williams at Argonne National Laboratory supports the measurement programs and develops new materials. The in-house synthesis of novel charge transfer organic superconductors and the chemical and electrochemical growth of very high purity polymeric organic conductors.

SANDIA NATIONAL LABORATORIES (continued)

Materials Chemistry - 03 -

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

281. CHEMICAL VAPOR DEPOSITION AND SURFACE PHOTOKINETIC RESEARCH

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

$435,000 03-3

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

SANDIA NATIONAL LABORATORIES
Livermore, CA 94550

Metallurgy and Ceramics - 01 -

D. L. Hartley - Phone (FTS) 532-2747 or (415) 422-2747

290. SURFACE LAYER EVOLUTION IN HIGH-TEMPERATURE DEPOSITION PROCESSES

M. Lapp, K. F. McCarty, R. J. Anderson.
Phone: (415) 422-2435
$300,000 01-1

Studies of the initial stages of deposition phenomena relevant to combustion and material processing environments. Utilize in situ, nonintrusive optical diagnostics to probe reactions at fluid/solid and solid/solid interfaces. Linear and nonlinear spectroscopies applied to dynamics of deposit layer evolution. Applications including combustion-flow deposits, high-temperature corrosion, materials joining, ceramic surface chemistry, and surface segregation.

291. GASES IN METALS/COMPUTATIONAL METALLURGY

M. I. Baskes, G. J. Thomas, M. S. Daw, S. M. Foiles, W. G. Wolfer, S. Robinson, S. Goods, C. F. Melius,
Phone: (FTS) 532-3226 or (415) 422-3226
$625,000 01-2

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

SANDIA NATIONAL LABORATORIES - LIVERMORE (continued)

292. THIN SURFACE LAYER REACTIONS

M. Lapp, R. J. Anderson, J. C. Hamilton, G. W. Foltz
Phone: (415) 422-2435

$240,000 02-2

Develop and evaluate advanced nonperturbing diagnostic techniques for high temperature materials research to produce in situ data. Focus on initial surface effects during exposures to combustion and materials processing environments. Real-time studies of species and reactions at interfaces including oxygen and hydrogen adsorption and surface segregation. Probing of surface and near-surface layers with Raman scattering, including capability to use micro-Raman spectroscopy with a hot stage. Nonlinear optical spectroscopies, in particular second harmonic generation, exploited to study surface processes at submonolayer coverages.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, CO 80401

C. Smith - Phone (FTS) 327-7180 or (303) 231-7180

Materials Research Branch - 01 -

D. Blake - Phone (FTS) 327-1202 or (303) 231-1202

295. POLYMER/THIN-FILM PHOTO AND CATALYTIC DEGRADATION RESEARCH

A. W. Czanderna, J. D. Webb, T. M. Thomas, J. R. Pitts
Phone: (303) 231-1240

$100,600 01-1

Photo and catalytic degradation mechanisms of polymeric materials exposed to simulated and enhanced solar environments in the presence and absence of supported thin films, stability of polymer/thin film interfaces, studies of polycarbonate and polypropylene in contact with copper oxide, silver, or gold, UV radiation, environmental oxidizing gases, and atmospheric pressures, interfacial catalytic effects and photodegradative effects, FT-IR reflection absorption spectroscopy, UV-vis spectroscopy, GPC, XPS, ISS, SIMS, AES, excimer/dye laser, solar simulator.

Solid State Research Branch - 02 -

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

296. SEMICONDUCTOR THEORY

A. Zunger
Phone: (303) 231-1172

$105,400 02-3

This project focuses on the application of first-principles band structure and total energy calculation techniques to the study of the electronic and structural properties of semiconductors, including the prediction of chemical trends and properties of new materials of potential photovoltaic interest, and the prediction of structural parameters and relative stabilities of these systems. The prototypical systems studied include: (i) disordered semiconductor alloys (e.g. $Si_x Ge_{1-x}$, $Ga_x In_{1-x}P$), (ii) novel ordered phases of alloys (e.g. SiGe, $GaInP_2$ $CdMnTe_2$), (iii) The Nowotny-Juza ternary semiconductors $A^{I}B^{II}C^{V}$ (e.g. LiZnAs), (iv) ternary chalcopyrites $A^{I}B^{III}C^{VI}_2$ (e.g. $CuInSe_2$) and (v) ternary pnictide $A^{II}B^{IV}C^{V}_2$ (e.g. $ZnSiP_2$). The theoretical tools used include: the total energy non-local pseudo-potential method and (b) the all-electron Mixed Basis Potential Variation band structure method. This work also includes the study of deep defects in semiconductors: e.g. chemical trends for 3d impurity levels in different host crystals (including alloys), prediction of hitherto unobserved impurity levels and excited states and understanding of the lattice distortions induced in the host, and the clarification of their likely impact on device characteristics. The theoretical technique used for the impurity studies is the Quasi-Band Crystal Field Green's function method.

STANFORD SYNCHROTRON RADIATION LABORATORY
Stanford University
P. O. Box 4349, Bin 69
Stanford, CA 94305

Solid State Physics - 02 -

A. I. Bienenstock - Phone (FTS) 461-9300 or (415) 854-3300, X 3153

298. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES

A. I. Bienenstock, G. S. Brown, H. Winick
Phone: (415) 854-3300 Ext. 3153

$1,140,000 02-2

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.

SECTION B

Grant Research

(Primarily Universities)

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

ARIZONA STATE UNIVERSITY
Tempe, AZ 85287

301. SURFACE STRUCTURES AND REACTIONS OF CERAMICS AND METALS

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

$104,250 02-2

Studies of surface structures of small crystals of oxides and metals and of the reactions of metals with oxides under the influence of intense ionizing radiation and heat using advanced electron optical techniques. High resolution electron microscopy, reflection electron microscopy, microdiffraction and electron energy loss spectroscopy conducted in high vacuum or ultra-high vacuum environments in which the specimen may also be prepared and treated. The oxide and metal specimens include samples with particle diameters <1nm important for catalyst systems and thin surface layers significant for bonding. Investigations of the effects of ionizing radiation and the presence of surface layers of water, oxygen or other gas. Excited states of small particles and the modification of the energetics as a function of the particle environment are also studied.

UNIVERSITY OF ARIZONA
Tucson, AZ 85721

302. ARTIFICIALLY LAYERED SUPERCONDUCTORS

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

$91,396 02-2

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

BATTELLE COLUMBUS LABORATORIES
Columbus, OH 43201

303. MULTIAXIAL STRESS RESPONSE OF CERAMICS

A. R. Rosenfield
Phone: (614) 424-4353
W. Duckworth
Phone: (614) 424-4230

$175,000 01-5

Response of ceramic materials to multiaxial stress states. Consideration of: (a) surface condition, (b) test geometry, and (c) environment. Control of each of the above variables so individual effects can be studied, specimen preparation to insure that the flaw population is isotropic and material directionality is eliminated. Relationship of stress-state effects to stress-intensity factor, effects of tensile and shear stresses parallel to an artificial crack and effects of stress ratios on strength in ceramic specimens containing natural flaws to evaluate statistical (Weibull) descriptions of strength. Material characterization, fractography, three-dimensional linear elastic finite element analysis of test-specimen geometries and stress-intensity factors. High-temperature biaxial tension tests of ceramic specimens containing controlled artificial flaws. Materials of interest: Al_2O_3, Si_3N_4, glass-ceramics, and partially stabilized ZrO_2.

BOEING AEROSPACE COMPANY
Seattle, WA 98124

304. X-RAY SPECTROSCOPIC INVESTIGATION OF METAMICTIZATION & ANNEALING IN CRYSTALLINE MATERIALS

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

$87,643 01-1

Detailed examination of number and kind of near neighbors about specific atoms and the near neighbor site geometries of metal atoms in metamict minerals as determined by extended X-ray absorption fine structure and X-ray absorption near edge structure (XANES) spectroscopy performed at the SSRL. Study of radiation damage annealing and leaching mechanisms of metamict minerals. Determination of the structure of the metamict state. Assessment of long-term stability of crystalline titanate, phosphate, and silicate radioactive wasteforms (e.g., SYNROC, Sandia Titanate, perovskite) which would be subject to the same processes of radiation damage and geochemical alteration in applications as a primary host for radioactive wastes.

BOSTON UNIVERSITY
Boston, MA 02215

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

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

$130,000 (16 Months) 02-2

Use of inelastic surface scattering of neutral atomic and molecular beams to investigate 1.) the different mechanisms for hydrogen exchange between particular crystal faces and the bulk and the relationship between these mechanisms and the rate of hydrogen uptake into the bulk in niobium, palladium, and tantalum, and 2.) energy exchange on transition metal crystal faces between rotational and translational excitations. A study of molecular hydrogen, deuterium, and hydrogen-deuterium beam scattering from the (100), (110), and (111) faces of iron and copper, prototypical of ferromagnetic and nonmagnetic metals.

BRANDEIS UNIVERSITY
415 South Street
Waltham, MA 02254

306. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

R. B. Meyer
Dept. of Physics
Phone: (617) 647-2231

$51,000 02-2

Experimental study of two-dimensional structures formed by interfacial and thin-layer colloids, especially with regard to two-dimensional melting. These colloidal systems exhibit truly two-dimensional behavior, free of periodic substrate interactions. The particle scale (0.1 to 10 um) permits both exploration of reciprocal space observations by coherent light scattering and direct real space observations by optical microscopy. Linear and two-dimensional aggregation of colloids driven respectively by an applied electric field and by salt addition. Continued development of a computerized image analysis system for studies of the pair correlation function which can be compared with theoretical predictions.

BRANDEIS UNIVERSITY (continued)

307. SYNTHESIS AND PROPERTIES OF NOVEL, ELECTROACTIVE ORGANOMETALLIC POLYMERS

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

$80,955 03-2

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

BRIGHAM YOUNG UNIVERSITY
Provo, UT 84602

308. INFLUENCE OF GRAIN BOUNDARY STRUCTURE DISTRIBUTION AND PROCESSING HISTORY ON INTERGRANULAR CREEP CAVITATION

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

$50,979 01-2

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

BROWN UNIVERSITY
Providence, RI 02912

309. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS

R. J. Asaro
Div. of Engineering
Phone: (401) 863-1456
J. Gurland
Div. of Engineering
Phone: (401) 863-2868

$61,838 01-2

This research involves experimental and modeling efforts addressing the deformation and fracture of various steels. Emphasis is placed on developing a detailed correlation between mechanical behavior and microstructural features in structural alloys, specifically regarding the limits of uniform ductility, necking strain and fracture toughness, shear localization at notch tips, propagation of surface cracks under fully plastic conditions, and hydrogen-enhanced void growth in steels deformed under different strain states.

310. CONCURRENT USE OF STRESS PULSES AND ULTRASONIC WAVES TO STUDY EFFECTS OF RAPID STRAIN ON THE INTERNAL STRUCTURE OF SOLIDS

C. Elbaum
Div. of Applied Mathematics
Phone: (401) 863-2186
A. Hikata
Div. of Applied Mathematics
Phone: (401) 863-2187

$105,500 01-2

Measurement of deformation of metals at intermediate strain rates (10^{-1}-10^{3}sec^{-1}), using the Hopkinson bar method for generating stress wave and ultrasonic methods to monitor the materials response, relationships between stress, mobile dislocation density, average velocity, and strain rate under single as well as multiple slip dislocation interaction with point effects, metals studied - Al, Fe, Nb, Ti, Zn.

BROWN UNIVERSITY (continued)

311. CHARACTERISTICS OF THE ROLE OF CYCLIC COMPRESSIVE LOADS IN THE GROWTH OF FATIGUE CRACKS IN STEELS

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

$98,768 01-2

Program will investigate the mechanics, mechanisms, and applications underlying the role of cyclic compressive loads in the growth of fatigue cracks in steels. To investigate the influence of continuous and periodic compression cycles on the propagation of cracks in constant and variable amplitude fatigue, in terms of the micro-mechanics of crack advance and crack closure, and to utilize the phenomenon of crack initiation under fully compressive cyclic loads for examining the progressive development of crack closure and for analyzing slow crack propagation rates. Will lead to a fundamental understanding of the role of compressive loads in the growth of fatigue cracks and will provide guidelines for fatigue design considerations in pressure vessel, piping and power generation applications, etc.

312. SURFACES AND THIN FILMS STUDIED BY PICOSECOND ULTRASONICS

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

$216,000 02-2

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

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA 91125

313. THE KINETICS OF SHORT RANGE ORDERING IN UNDERCOOLED ALLOYS

B. T. Fultz
Materials Science Department
Phone: (818) 356-2170

$80,700 01-1

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

314. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

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

$275,000 01-1

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

315. MELTING IN ADSORBED FILMS

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

$102,199 02-2

Study of adsorbed films by thermodynamic methods, combining heat capacity and vapor pressure measurements on a systematic grid of points in the coverage (N) versus temperature (T) plane. From these measurements the appropriate thermodynamic free energy may be constructed as a function of its proper variables N and T, and from the tabulated free energy all thermodynamic quantities (i.e. entropy, compressibility, etc.) may be obtained. Pulsed NMR studies of the dynamics to supplement the thermodynamic measurements, particularly for features for which the latter are inconclusive or insensitive.

UNIVERSITY OF CALIFORNIA/DAVIS
Davis, CA 95616

316. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY

A. K. Mukherjee
Dept. of Mechanical Engineering
Phone: (916) 752-1776, 0580

$31,300 01-2

Experimental study of superplastic deformation of metals, microduplex steels and Al-base alloys, correlation between mechanical behavior (e.g., stress, strain rate, temperature) and microstructure (e.g., grain size, dislocation structure and precipitate morphology), identification of superplastic and creep mechanisms, analysis of cavitation behavior and its implication to superplastic forming.

317. CHEMICAL DECOMPOSITION OF CERAMICS UNDER IRRADIATION

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

$71,000 (6 months) 01-4

Investigation of electron and ion irradiation induced ionization, displacement damage, diffusion, and stimulated desorption by means of in situ electron microscopy and mass spectroscopy. Study of ion mixing effects under ion irradiation. Finite difference solutions to a two-dimensional diffusion equation for the irradiation and desorption process. Materials: Na- Al_2O_3, Na borosilicate glass, TiC.

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

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

$100,291 01-5

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

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, CA 92717

319. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

J. C. Hemminger
Dept. of Chemistry
Phone: (714) 833-6020
S. Ushioda
Dept. of Physics
Phone: (714) 833-6619

$162,500 02-2

Inelastic light scattering spectroscopy and modern surface science technology combined in investigations of the binding and chemistry of adsorbates on well characterized surfaces. Experiments to elucidate the mechanism of the "surface" enhanced Raman scattering phenomena, and to determine the range of applicability of unenhanced Raman scattering to adsorbate studies. Adsorbate Raman spectra of evaporated metal substrates (Ag on mica and Ag on other transition metals). Raman enhancement correlated with the electronic energy levels of the metal-adsorbate system, determined by high resolution electron energy loss spectroscopy and photoemission studies. Inelastic light scattering studies: molecular adsorbates, such as tetracyanoethylene (TCNE) and tetracyano-quinodimethane (TCNQ), which exhibit strong charge transfer on bonding to surfaces; and polymer film formation in the TCNE and TCNQ - metal systems.

320. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

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

$106,592 02-3

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/LOS ANGELES
Los Angeles, CA 90024

321. AMORPHIZATION OF METALLIC ALLOYS UNDER PROTON AND NEUTRON IRRADIATION

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

$102,934 01-4

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

322. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

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

$180,000 02-5

Investigation of non-linear, non-equilibrium properties of materials and the properties of quantum fluids as follows: (1) the excitation, observation, and function of mesoscale objects in molecular solids using optical, ultrasonic, and microwave techniques at low temperatures and with special attention to the implications for non-linear natural engines. (2) Acoustical models of non-linear vibrational systems, especially as they illuminate the mesoscale systems problem. (3) Non-linear dynamical properties of convecting dilute solutions of ^3He in superfluid ^4He, with primary emphasis on time-dependent properties, but with new attention to pattern formation and to the effect of geometry. (4) Non-linear dynamical properties of a driven two-dimensional plasma of helium ions under the surface of liquid helium. (5) Properties of superfluid ^3He, especially questions relating to the A->B phase transition and to magnetic properties. (6) Properties of spin-polarized hydrogen isotopes, especially experiments on the magnetoacoustic effect and their consequences for transport in atomic hydrogen and deuterium.

UNIVERSITY OF CALIFORNIA/SAN DIEGO
La Jolla, CA 92037

323. INVESTIGATION OF SUPERCONDUCTIVITY AND MAGNETISM IN D- AND F-ELECTRICAL MATERIALS

M. B. Maple
Dept. of Physics
Phone: (619) 452-3969

$336,378 02-2

An investigation of superconductivity and magnetism and the interaction of these phenomena in binary and ternary transition metal, rare earth and actinide compounds. Emphasis on RRh_4B_4, R being a rare earth, where superconductivity and long range magnetic order are known to exist, and on heavy fermion systems. A search for superconducting and unusual semi-conducting compounds of cerium and uranium. Changes in superconducting and magnetic properties of compounds prepared by nonequilibrium techniques such as shock compression.

324. ION MIXING AND SURFACE MODIFICATION IN METAL SEMICONDUCTOR SYSTEMS

S. S. Lau
Dept. of Electrical Engineering and Computer Sciences
Phone: (619) 452-3097
D. M. Scott
Dept. of Electrical Engineering and Computer Sciences
Phone: (619) 452-3428

$200,845 (15 months) 02-4

Investigation of the physical mechanisms responsible for ion-mixing effects in metal-semiconductor systems. Generalize and predict ion-induced reactions, correlations between ion-induced reactions and those induced by conventional thermal annealing. Physical mechanisms and conditions necessary for the formation of a specific reaction product determined. Different metal-silicon systems investigated. Sample configurations include metal layer on silicon bilayers, multi-layers, and alloy thin film structures. Primary experimental tools: ion implantation, thermal annealing, Rutherford backscattering, Auger electron spectroscopy, X-ray diffraction, and transmission electron spectroscopy. A collaborative program between the University of California, San Diego, and Cornell University including interaction with Oak Ridge National Laboratory.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, CA 93106

325. CONDENSED MATTER RESEARCH USING THE UCSB FREE ELECTRON LASER

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

$115,500 02-2

Initiate the first use of a Free Electron Laser (FEL) for materials research in the United States. This unique device is a source of high intensity, coherent, but pulsed electromagnetic radiation tunable over the wavelength range 100 to 1000 micrometers. Research on nonlinear phenomena involving phonons, magnons, and other excitations of ordered and disordered materials. Use of techniques such as two-photon spectroscopy following development of facilities and instrumentation.

326. RESEARCH ON PATTERN FORMATION IN SYSTEMS FAR FROM EQUILIBRIUM

J. S. Langer
Dept. of Physics
Phone: (805) 961-4111

$107,975 02-3

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

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

327. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino
Physics Dept.
Phone: (805) 961-2871
J. R. Schrieffer
Physics Dept.
Phone: (805) 961-2280
R. L. Sugar
Physics Dept.
Phone: (805) 961-3469

$113,384 02-3

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

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

328. THE EFFECT OF STRESS ON PRECIPITATE MORPHOLOGY

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

$107,651 01-1

Theoretical and experimental study of second phase morphology changes, owing to misfit strains and applied stress. System parameters include misfit strains, volume fraction, nature of applied stress, differences in elastic constants. Theoretical approach uses bifurcation theory. Ni-Al alloys are being studied; future studies will also be on Ni-(Ti,Al)-(Cr,Mo). Experimental techniques include electron microscopy and X-ray diffraction.

CARNEGIE MELLON UNIVERSITY (continued)

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

I. M. Bernstein
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2700
A. W. Thompson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2711
G. W. Warren
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 268-2700

$114,314 01-2

Effects of microstructure and nature of passive surface films on corrosion fatigue crack initiation, heat treatment developed to change the microstructure and thus the degree of slip planarity in A286, a superalloy stainless steel, potentiostatic and potentiodynamic techniques used to demonstrate that the alloy forms a stable passive film in various aqueous solutions, highly resistant to pitting, repassivation kinetics determined in scratch tests, electrochemical results are being analyzed using existing and developed current buildup and decay models, experiments underway to measure fatigue-induced crack initiation rates under controlled electrochemical conditions, comparing these to similar tests run in air and in inert environments.

CASE WESTERN RESERVE UNIVERSITY
Cleveland, OH 44106

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

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

$149,110 01-2

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

UNIVERSITY OF CHICAGO
5801 S. Ellis Avenue
Chicago, IL 60639

331. RESEARCH IN THE THEORY OF CONDENSED MATTER AND ELEMENTARY PARTICLES

L. P. Kadanoff
The James Franck Institute
Phone: (312) 962-7189
Y. Nambu
The James Franck Institute
Phone: (312) 962-7286
D. Friedan
Dept. of Physics
Phone: (312) 962-7119
S. Shenker
Dept. of Physics
Phone: (312) 962-7187

$185,000 02-3

Theoretical research on problems relevant to quantum field theory and statistical mechanics. Topics to be considered: conformal field theory and two dimensional critical phenomena, formation of macroscopic structures in dynamical systems (pattern formation), the exact chiral symmetry in lattice fermion theories, string theory and random surfaces in high energy physics and statistical mechanics, and fermion-boson mass relations in Bardeen-Schrieffer-Cooper type theories.

UNIVERSITY OF CINCINNATI
Cincinnati, OH 45221

332. SURFACE CHEMISTRY OF ELECTROCATALYSIS

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

$81,000 03-2

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

CLARK COLLEGE
Atlanta, GA 30314

333. INVESTIGATIONS OF CHARGE TRANSPORT IN THE THERMOELECTRET STATE OF SOME GLASSES AND CERAMICS

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

$79,650 01-3

Investigation of the mechanism of formation and decay of electrets in nonpolar inorganic polycrystalline and amorphous dielectrics. Experimental characterization of electret formation with sample temperature, polarization field, and cooling rate, and of electret decay in the open and closed circuit condition. Extension of Swann-Gubkin theory by considering the nonpolar part of electret polarization through the displacement of ions to account for the production of nonpolar electrets. Materials of interest include $CaTiO_3$, $SrTiO_3$, BaO_4, TiO_2, $BiTiO_3$, $(SrBi)TiO_3$, chalcogenide glasses and elemental Se. X-ray diffraction. Thermally stimulated discharge current analysis.

COLORADO SCHOOL OF MINES
Golden, CO 80401

334. PHYSICAL METALLURGY OF FERROUS ALLOY WELD METAL

D. L. Olson
Dept. of Metallurgical Engineering
Phone: (303) 273-3787
D. K. Matlock
Dept. of Metallurgical Engineering
Phone: (303) 273-3775

$175,118 (13 months) 01-5

Evaluation of microstructures and properties of new compositional grades for multipass austenitic weld metal for low and high temperature applications. Alloy modifications, including substitutions for chromium. Expressions for predicting as-solidified weld metal microstructures extended to include effects of composition gradients. Evaluation of effects of compositional and microstructural gradients on thermal stability and mechanical properties of modified austenitic weld metals in both single and multipass weldments.

COLORADO SCHOOL OF MINES (continued)

335. PHOTON SCATTERING AND INTERACTION ANALYSIS OF INTERFACIAL CORROSION AND CATALYSIS

T. E. Furtak
Dept. of Physics
Phone: (518) 266-6454

$42,977 02-2

Use of optical phenomena to investigate microscopic effects at the electrolyte-solid interface surface vibrational spectroscopy studies of the non-enhanced and enhanced Raman effect. Elucidate electronic structure by spectroscopic ellipsometry. Nonlinear surface effects giving rise to surface second harmonic generation. Use of metallic overlayers as prototypical strongly bound adsorbates.

COLORADO STATE UNIVERSITY
Fort Collins, CO 80525

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

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

$72,423 02-3

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

UNIVERSITY OF COLORADO
Boulder, CO 80309

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

W. O'Sullivan
Dept. of Physics
Phone: (303) 492-7457
R. Mockler
Dept. of Physics
Phone: (303) 492-8511

$123,000 02-2

Preparation and study of systems of synthetic colloidal microspheres that exhibit the primary phenomena of physical interest in lower dimensional systems. Use of e-beam lithography and film deposition for construction of substrate particle-traps in extended or local patterns, to provide potential fields acting on the colloidal particles. Quasi-elastic light scattering microscopy 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 equivalent of ultra high pressures, experimental and computer simulation of collapse of particle distributions on quenching electrostatic interparticle forces, critical diffusion rates in thin binary liquid films.

COLUMBIA UNIVERSITY
New York, NY 10027

338. PROTONIC AND OXYGEN-ION CONDUCTION IN SOLID OXIDE ELECTROLYTES

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

$132,837 01-3

Ion transport processes in perovskite-structured oxides which can be converted into high-temperature protonic conductors by treatment in water vapor. Determination of the manner in which protons enter the host crystal and the appropriate kinetic parameters (e.g., activation energies and association energies) that determine the rate of migration. Monitoring of proton content by observation of intensity of infrared absorption due to the OH^- stretching mode. Investigative techniques include ionic conductivity (complex impedance as a function of frequency), diffusion measurements (including H <-> D interchange), dielectric and anelastic relaxation, electrolyte cell measurements, EPR, NMR, and HADES type computer simulations. Materials of investigation: single crystal $KTaO_3$, sintered polycrystal $SrCeO_3$, $SrTiO_3$, and other perovskite oxides.

UNIVERSITY OF CONNECTICUT
Storrs, CT 06268

339. THE FATIGUE BEHAVIOR OF FERRITIC STEELS AT ELEVATED TEMPERATURES

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

$55,508 01-1

The influence of creep and oxidation on the rate of fatigue crack growth in ferritic steels. Evaluation of the fatigue behavior of alloys with large and short cracks (relative to the grain size) in steels having bainitic, martensitic, and duplex martensitic-ferritic microstructures. Both wrought and welded structures are investigated.

340. ELECTRODE STUDIES IN MOLTEN SALTS

O. F. Devereux
Dept. of Metallurgy
Phone: (203) 486-4620

$11,143 01-3

Deterioration of refractory oxide films on Ni and Fe in sulfide-bearing molten salts. Field and anion effects, 'electrochemical' dissolution of oxides. Film thinning, pore formation, and structure change evaluation by impedance techniques. Formation of anodic chromium sulfides in molten sulfide salts. Current-potential characteristics of anodic sulfide films.

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

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

$91,600 02-2

Investigation of four aspects of the interaction of single or multiple optical fields with a rare earth ion and its host matrix to elucidate the non-linear optical properties and energy transfer in the system. These aspects are: the optical gain and loss in Ce^{3+}:$LiYF_4$; the non-radiative relaxation processes and the ion-lattice interactions associated with the 5d->4f transition; photoconductivity due to excited states of rare earth ions in crystals and glasses; and phase conjugate wave generation and laser-induced grating studies at near ultraviolet wavelengths.

CORNELL UNIVERSITY
Ithaca, NY 14853

342. THE MIGRATION OF GRAIN BOUNDARIES IN CERAMICS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

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

$112,000 01-1

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic-covalent solids. Concerns include (1) misorientation between grains and boundary plane orientation, (2) geometry of interfacial dislocations and steps, (3) interfacial chemistry including local segregation and nonstoichiometry, and (4) interfacial pinning by pores or crystalline or amorphous pockets or films of a second phase. Materials of investigation include Al_2O_3, MgO, NiO, Mg-Al spinel, Si, Ge, Si_3N_4, and SiC. Studies on both powder compacts and bicrystals involve visible light microscopy, electron microprobe analysis, and strong- and weak-beam, lattice fringe, X-ray energy dispersive, and electron energy loss TEM analysis.

343. EXPERIMENTAL AND THEORETICAL STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES

S. L. Sass
Dept. of Materials Science and Engineering
Phone: (607) 255-5239
N. W. Ashcroft
Dept. of Physics
Phone: (607) 255-3309

$289,868 01-1

Investigation of grain boundary structure of BCC metals, ceramics, and intermetallic compounds using transmission electron microscopy and electron diffraction, and X-ray diffraction techniques, study of the influence of segregation on the structure of grain boundaries in Fe-base alloys, MgO + Fe and Ni_3Al, determination of grain boundary region in order to obtain structural information, study theoretically the structure of crystalline defects including grain boundaries, and the interatomic potentials needed to calculate their structure.

CORNELL UNIVERSITY (continued)

344. AN INVESTIGATION OF MECHANICAL BEHAVIOR OF POLYCRYSTALLINE SOLIDS

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

$192,400 01-2

State-variable descriptions of nonelastic deformation and related phenomena in polycrystalline solids. Extensive use is made of load relaxation experiments and of combinations of load relaxation and stress-dip experiments spanning strain rates from 10^{-8} to $10^{2}.s^{-1}$ and low to high ($T > T_m/2$) homologous temperatures. Efforts to relate microstructurally or physically based theories to various state variables are embodied in the program as well as parallel efforts to incorporate these constitutive relations into complex stress, deformation, and structural design analyses.

345. EXPERIMENTS AND MICROMECHANICAL MODELS FOR CREEP-RUPTURE IN POLYMER-MATRIX COMPOSITES

S. L. Phoenix
Sibley School of Mechanical and Aerospace Engineering
Phone: (607) 255-3462

$121,361 01-2

Basic research will include both experimental and modeling tasks with goals to predict failure times of continuous-fiber reinforced polymer composites under load and relate the mean lifetime to fiber and matrix properties. Theoretical effort using probabilistic statistics to derive a distribution of composite strengths; will incorporate distributions of individual fiber strengths and flaws in the composite, local load sharing rules around initial flaws, and viscoelastic properties of the matrix. Experimental effort will involve creep-rupture testing of "microcomposites" to evaluate the models.

CORNELL UNIVERSITY (continued)

346. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF CERAMICS

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

$105,410 01-2

Role of inhomogeneities (both second phases and agglomerates) and shear strain in the densification of powder. Elucidation of the mechanisms of densification and flaw generation during high-temperature processing of TiO_2 and TiO_2-Al_2O_3 powder compacts with inhomogeneous microstructures. Influence of agglomerates, non-uniform packing, and second phase constituents on the densification process. Measurement of sintering pressure. Free sintering, hot-pressing, and sintering under superimposed hydrostatic pressure experiments on TiO_2 on Al_2O_3 (model material for dry processing) and Si_3N_4 (with a liquid phase additive for wet processing). Colloidal processing of powder.

CORNELL UNIVERSITY (continued)

347. DEFECT STUDIES IN III-V THIN FILM SEMICONDUCTORS

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

$110,000 01-3

Study the correlation between the electronic properties, atomic structure, and local chemistry of defects in GaAs, GaAs-based ternaries and at the interface between GaAs, GaAs-based ternaries and Si. The main objectives of the proposed research:

(1) Clarify the core structure of clean and decorated defects. Investigate relation between decoration state and electrical activity using a combination of TEM, in situ EBIC, CL, PL, and DLTS. Particular emphasis is placed on interface dislocations in multilayer structures.

(2) Investigate changes in the electrical activity and structure of defects as a function of annealing conditions using capped anneals, non-capped anneals (vacuum), annealing with InGaAs (J. Woodall method) and annealing under very slow CVD growth conditions.

(3) Investigate the structure of grain boundaries, with particular attention to the possible dissociation of asymmetric grain boundaries into subsets of symmetric boundaries. Study the electrical activity of such boundaries and the correlation with structure, especially symmetry. Identify annealing treatments which minimize the electrical activity of boundaries.

(4) Investigate the electrical activity of anti-phase boundaries in GaAs on Si and Ge as a function of their structure.

(5) Investigate the origin of CL contrast of Si-GaAs and its connection to the spatial variation of deep states, using a combination of EBIC, CL, TEM, and spatially resolved PL.

CORNELL UNIVERSITY (continued)

348. INTERFACE SCIENCE AND ENGINEERING 87--AN INTERNATIONAL CONFERENCE ON THE STRUCTURE, PROPERTIES, AND PROCESSING RELATIONSHIPS OF INTERNAL INTERFACES

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

$5,000 01-3

International symposium to be held on internal interfaces. Fundamental aspects of the structure, phase equilibria, mechanical properties, electronic and thermal properties of internal interfaces will be examined and the feasibility of processing approaches to control interface structure will be explored.

349. STRONGLY INTERACTING FERMION SYSTEMS: EMPHASES ON HEAVY FERMIONS

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

$120,000 02-3

Theory of heavy fermion behavior in lanthanide and actinide compounds, and more generally of systems with f and/or d electrons that are strongly interacting or correlated. Aims at understanding the occurrence or absence of heavy fermions in such systems, the nature of the low temperature coherent state and the transition to a Kondo-like state at higher temperatures, and of course, at an account of the unusual magnetic and superconducting properties of heavy fermion. Extension to magnetically concentrated systems of approaches known from experience with magnetically dilute alloys, including renormalization study of two-impurity models. Close interaction with ongoing experimental programs at DOE laboratories and elsewhere. Exploration and development of new theoretical and computational methods, for example utilizing functional-integral formulations, discretizing on a lattice in space and temperature, renormalization transformations, and Monte Carlo technique with a Langevin equation for non-perturbative calculation of properties.

DARTMOUTH COLLEGE
Hanover, NH 03755

350. THE ROLE OF GRAIN BOUNDARIES ON THE STRENGTH, DUCTILITY, AND TOUGHNESS OF $L1_2$ INTERMEDIATE COMPOUNDS

E. M. Schulson
Thayer School of Engineering
Phone: (603) 646-2184

$124,430 01-2

Examine dislocation pileup/grain boundary accommodation model in more detail, carry out systematic in situ TEM deformation studies on Ni-rich, stoichiometric and Ni-lean Ni_3Al both with (0.35at%) and without boron; investigate grain boundary sliding in Ni_3Al by systematic experiments on the effects of grain size on high-temperature deformation (800-1200K) of NI_3Al with (0.35at%) and without boron; investigate grain size effects on the strength and ductility of Ni_3Si by systematic experiments on the effects of grain size on the mechanical properties and resultant deformation structure; improve the toughness of Ni_3Al through grain shape control, i.e., generate equiaxed fine grain structure with simultaneous increase of aspect ratio, comparative tests (fibrous vs. equiaxed microstructures) performed at RT using Charpy impact technique. Subsequent fracture toughness measurements using standard ASTM procedures.

UNIVERSITY OF DELAWARE
Newark, DE 19716

351. DURABILITY OF SHORT FIBER COMPOSITE MATERIALS

T.-W. Chou
Dept. of Mechanical and Aerospace Engineering
Phone: (302) 451-2904

$49,742 01-2

Experimental and theoretical investigation of the durability of short glass and carbon fiber reinforced thermoplastics, strength and fracture behavior of fiber bundle, resin matrix and composites subjected to static and cyclic loadings as well as aggressive environmental attack, measurements of residual strength, failure time and failure characteristics of aligned and partially aligned short fiber composites, characterization of stress-corrosion cracking, fatigue, and corrosion fatigue, determination of fiber-matrix interfacial profile from fracture surface analyses, analytical modeling of the stress-corrosion behavior of fiber bundles and resin matrices, and development of a statistical strength theory for fiber composites, major parameters in analysis include fiber flaw induced stress concentration and concentration of corrosive agents, correlation of experiments with modeling.

UNIVERSITY OF DELAWARE (continued)

352. NEUTRON STUDIES OF LIQUID AND SOLID HELIUM

H. R. Glyde
Dept. of Physics
Phone: (302) 738-2661

$ 67,340 02-1

Theoretical calculations of properties of liquid and solid helium for direct comparison with neutron measurements. The aim is to interpret neutron scattering data, to investigate implications of experiments in terms of extant and new models, and to propose new experiments. Specific examples are: direct calculation of the dynamic form factor S(Q,) in liquid ^{3}He for comparison with existing data to test models of the effective interactions between atoms in the liquid, calculations of the momentum distribution in liquid ^{3}He and in solid ^{4}He for comparison with experiments at IPNS(ANL), and to test the impulse approximation using models appropriate to solid ^{4}He. Development of a microscopic theory of liquid ^{3}He based on Green's function methods (a long term project).

UNIVERSITY OF DENVER
Denver, CO 80208

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

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

$69,911 01-2

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

UNIVERSITY OF DENVER (continued)

354. DETECTING AND MONITORING CRACK INITIATION AND GROWTH IN AUSTENITIC AND FERRITIC STEELS

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

$69,520 01-5

The objective of this research is to access the degree to which crack nucleation and growth in steels can be quantitatively detected and characterized by two nondestructive methods, the modulus defect and acoustic emission (AE). Mechanical tests will be conducted with steels treated to yield specific microfracture mechanisms in various environments and strain states. The correlation of the measured AE with specific sources in the material will be sought in an effort to determine the uniqueness of AE signatures.

FLORIDA STATE UNIVERSITY
Tallahasee, FL 32306

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

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

$125,060 02-2

Construction of a He atom-surface scattering instrument and the study of the dynamics of crystalline surfaces by low energy He-atom scattering. Extraction from surface phonon data of information on the interactions between surface species and hence on their physical and chemical properties. Surface phonon dispersion curves obtained by time-of-flight methods from inelastic single atom-surface encounters. Corrugation of and energy levels in the He-surface potential, obtained from elastic specular and diffractive scattering. Information on relaxation phenomena obtained from measurements of phonon lifetimes. Studies envisaged include: (110) surfaces of Au, Pt, and Ir, which reconstruct as a function of temperature. Surfaces of active metals (Ni, Cu), both clean and with physisorbed or chemisorbed layers. Surface phonon anomalies in high Tc 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

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

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

$66,631 01-3

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

357. MODERATE AND LOW TEMPERATURE OXIDATION OF CLEAN NICKEL, CHROMIUM, AND Ni-Cr ALLOYS

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

$123,136 01-3

Investigation of low and moderate temperature ($100^{o}K < T < 800^{o}K$) oxidation of atomically clean single and polycrystalline Ni, Cr, and Ni-Cr alloys. Surface segregation studies by Auger electron, X-ray photoelectron and ion scattering spectroscopies. Oxidation kinetics and adsorbed states characterization in ultra-high vacuum (UHV) with X-ray photoelectron spectroscopy, scanning Auger electron spectroscopy, low energy and reflection high-energy electron diffraction (LEED and RHEED), work function changes and temperature desorption spectroscopy. Oxide structure analysis with LEED, RHEED, and transmission electron microscopy. The oxygen pressure will be varied from 10^{-10} Torr to 1 atmosphere, with higher pressure exposures being accomplished in a reaction chamber external to the UHV chamber. Specific aspects of the oxidation to be studied include oxide nucleation, lateral oxide growth to form a coalesced layer, thickening of the coalesced oxide layer, dissolution of the oxygen into the bulk and the effect of controlled oxide microstructure upon high temperature oxidation. This study will directly investigate the phenomena occurring in the transition from an atomically clean surface to a thick oxide at elevated temperatures.

UNIVERSITY OF FLORIDA (continued)

358. IMPLANTATION STUDIES OF HYDROGEN BY FIELD-ION MICROSCOPY AND SPECTROSCOPY

J. J. Hren
Dept. of Materials Science and Engineering
Phone: (904) 392-6985

$80,025 01-3

This research is directed towards understanding the properties of hydrogen in Fe, Ta, and Ni by field ion microscopy (including the imaging atom probe) and electron microscopy. Hydrogen, deuterium, and/or helium ions are to be implanted into specimens in situ at cryogenic temperatures; diffusivities of H(D) and He will be measured by monitoring the evolution of these species through field desorption. Transmission electron microscopy (TEM) will be used to check many of the FIM results.

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

M. D. Sacks
Dept. of Materials Science and Engineering
Phone: (904) 392-6676
J. W. Williams
Dept. of Materials Science and Engineering
Phone: (904) 392-6698
C. D. Batich
Dept. of Materials Science and Engineering
Phone: (904) 392-6630

$114,863 01-3

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

UNIVERSITY OF FLORIDA (continued)

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

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

$78,000 02-2

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

361. STUDIES OF HEAVY FERMION SYSTEMS

G. R. Stewart
Dept. of Physics
Phone: (904) 392-9263, 0521

$185,000 02-2

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

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

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

$98,008 03-1

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

GEORGIA TECH RESEARCH CORPORATION
Atlanta, GA 30332-3368

363. A STUDY OF MECHANISMS OF TIME-DEPENDENT CRACK GROWTH AT ELEVATED TEMPERATURE

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

$104,179 01-2

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

364. CRYSTALLINE METAL-SEMICONDUCTOR SUPERLATTICES

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

$125,000 02-2

Emphasis on the growth of LaTe/PbTe superlattices using metallorganic chemical vapor deposition techniques. Superlattice characterization by secondary ion mass spectroscopy, X-ray diffraction, optical spectroscopy and electrical transport techniques. The goal is to develop a growth process for superior superlattice materials which can be used with reproducible results. The conducting and superconducting (if any) properties of LaTe/PbTe superlattices will be examined.

365. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND THE GEOMETRY OF SURFACE CLUSTERS

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

$181,000 02-3

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

GEORGIA TECH RESEARCH CORPORATION (continued)

366. LOCAL MANY-BODY EFFECTS IN THE OPTICAL RESPONSE OF NARROW BAND SOLIDS

A. Zangwill
Dept. of Physics
Phone: (404) 894-7333
D. Liberman
Lawrence Livermore National Laboratory
Phone: (415) 423-0505

$53,782 02-3

Calculation of photoelectric partial cross sections that apply realistically to narrow band solids, e.g. to late 3d transition metals, cerium, light actinides, and to intermetallic compounds of all of these. Such calculations are not now available and will supply essential guidance to the interpretation and planning of experiments involving measurement of photoabsorption and photoemission at energies near core and deep core thresholds. Both atomic and solid state many-body effects will be incorporated in treatment of an embedded cluster model. The computational method combines RPA-like extension of density functional theory, self-consistent multiple-scattering techniques, and final-state wave functions calculated in the presence of a core hole. Special care will be accorded to the interplay between dielectric and core-hole many-body effects, both of which are expected to be important in the materials of interest.

367. A CARBANION APPROACH TO POLYACETYLENE

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

$73,000 03-1

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

HARVARD UNIVERSITY
Cambridge, MA 02138

368. DRIFT MOBILITIES BY TIME-OF-FLIGHT METHODS AND TIME-DEPENDENT PHOTOTRANSPORT IN THE NANOSECOND REGIME IN AMORPHOUS SEMICONDUCTORS

W. Paul
Div. of Applied Sciences
Phone: (617) 495-2853

$130,000 02-2

Time-of-flight measurements in the nanosecond to millisecond regime, and other time-dependent studies of amorphous hydrogenated silicon, and undoped, which have been carefully characterized as to their structure, band structure and steady-state electrical and optical properties. A coherent, self-consistent model of transport and recombination processes sought.

369. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

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

$229,000 02-2

Investigation of the fundamental physical properties of spin-aligned atomic hydrogen and deuterium at very low temperatures in the gaseous phase and adsorbed on the liquid and films of helium. Attempts to reach the Einstein Bose condensation in these three and two dimensional systems. Development of a cryogenic maser utilizing spin aligned atomic hydrogen as an improved frequency standard (clock).

UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE
Chicago, IL 60680

370. CORROSION OF IRON, NICKEL, AND COBALT-BASED ALLOYS IN ENVIRONMENTS CONTAMINATED WITH CHLORINE

M. McNallan
Dept. of Civil Engineering, Mechanics and Metallurgy
Phone: (312) 996-2436

$38,495 01-3

This project addresses corrosion of structural alloys in mixed gases. Emphasis will be placed on elucidating the effects of (1) alloying elements Cr and Al on the corrosion behavior of Fe-, Co-, and Ni- base alloys, (2) transients in the O_2 and Cl_2 potentials during corrosion, and (3) additions of S (as SO_2) as a third oxidizing species during corrosion.

INDIANA UNIVERSITY
Bloomington, IN 47402

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

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

$82,896 (15 months) 02-2

Measurements of surface vibrational properties of clean surfaces and of metal-adsorbate systems principally by high-resolution [3-7 meV] electron energy loss spectroscopy. Detailed phonon dispersion information to be obtained on a variety of metal surfaces e.g., palladium, aluminum, copper and gold, and adsorbate elements, such as oxygen. Study of the interaction between metal atoms at surfaces and the modifications which accompany adsorption phenomena.

KANSAS STATE UNIVERSITY
Manhattan, KS 66506

372. MAGNETIC STUDIES OF IRON:RARE-EARTH:METALLOID ALLOYS

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

$43,960 02-2

Investigation of the new iron:rare-earth:metalloid alloys with high potential for permanent magnetic applications including $Fe_{77}R_{15}M_8$ and $Fe_{82}R_{12}M_6$ where R is primarily a rare-earth and M is a metalloid such as B, C, and Si. Main emphasis on preparation techniques, correlation of magnetic properties of 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 the University of Nebraska.

UNIVERSITY OF KENTUCKY
Lexington, KY 40506

373. STUDIES OF THE MICROSCOPIC PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE INTERCALATION COMPOUNDS

P. C. Eklund
Dept. of Physics and Astronomy
Phone: (606) 257-6719

$142,000 (15 months) 02-2

Investigation of chemical and physical properties of well-staged graphite intercalated compounds (GIC). Study of the electronics, lattice dynamical (Raman and Infrared studies) and structural properties of donor- and acceptor-type GIC's. Optical reflectance measurements over range 0.05 - 10 eV, and X-ray diffraction studies. Extensive and on-going collaborations with scientists at other institutions on complementary Mossbauer spectroscopic and neutron scattering research.

374. STRUCTURAL AND SURFACE CHARACTERIZATION OF DISPERSED METAL CATALYSTS

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

$87,892 03-3

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

LEHIGH UNIVERSITY
Bethlehem, PA 18015

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

C. E. Lyman
Dept. of Metallurgy and Materials Engineering
Phone: (215) 861-4249

$71,847 01-1

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

376. ANALYTICAL ELECTRON MICROSCOPY STUDIES OF PRECIPITATION IN CERAMIC SYSTEMS

M. R. Notis
Materials Research Center
Phone: (215) 861-4225
D. B. Williams
Materials Research Center
Phone: (215) 861-4220
M. P. Harmer
Materials Research Center
Phone: (215) 861-4220

$130,000 01-1

Study of precipitation phenomena by means of analytical and high resolution electron microscopy, laser Raman spectroscopy and X-ray diffraction. Phase transformations resulting in transformation toughening in ZrO_2 containing ceramics. Precipitate dissolution kinetics and transient second phase phenomena in the Y_2O_3-La_2O_3 system. Precipitate coarsening kinetics in NiO and CoO, and precipitation processes in mullite and glass ceramic materials.

LEHIGH UNIVERSITY (continued)

377. THE EFFECT OF POINT DEFECTS ON STRUCTURAL PHASE TRANSITIONS

J. Toulouse
Dept. of Physics
Phone: (215) 861-3960

$87,000 01-1

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

378. INVESTIGATIONS OF CREEP CAVITATION IN TYPE 304 STAINLESS STEEL

T. Delph
Dept. of Mechanical Engineering & Mechanics
Phone: (215) 861-4119

$74,060 01-2

Experimental studies of creep cavitation in austenitic stainless steel under uniaxial and multiaxial stress states using automatic image analysis, creep cavitation around notches, statistical analysis of cavitation data, stereological considerations.

379. CORROSION FATIGUE OF SMALL CRACKS: MECHANICS AND CHEMISTRY

R. P. Wei
Dept. of Mechanical Engineering and Mechanics
Phone: (215) 861-3587

$151,180 01-2

Experimental and theoretical study of corrosion fatigue of NiCrMoV and 304 stainless steels in aqueous solutions, kinetics of growth of small fatigue cracks as a function of frequency, solution chemistry, temperature and crack length, electrochemical reaction kinetics as a function of temperature in the same environment, relating fatigue crack growth response to the electrochemical reaction kinetics, modeling of electrochemical conditions near the crack tip and of the electrochemical and micromechanics aspects of small-crack growth.

LEHIGH UNIVERSITY (continued)

380. GRAIN BOUNDARY DIFFUSION IN ORIENTED Ni_3Al BICRYSTALS CONTAINING BORON

Y-T. Chou
Division of Metallurgy and Materials Engineering
Phone: (215) 861-3020

$83,530 01-3

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

UNIVERSITY OF MARYLAND
College Park, MD 20742

381. GASES ON METAL SURFACES: ADSORPTION AND PHASE TRANSITIONS

T. L. Einstein
Dept. of Physics
Phone: (301) 454-3419
R. E. Glover III
Dept. of Physics
Phone: (301) 454-3417
R. L. Park
Dept. of Physics
Phone: (301) 454-4127

$ 39,100 02-2

Joint theoretical/experimental investigation of surface interactions and imperfections which have an important influence on surface reactivity. Studies of oxygen and carbon monoxide adsorption and reaction at low temperatures on polycrystalline films and single crystal surfaces. Controlled variation of substrate and beam temperatures to probe reaction barriers. Measurements of adatom-adatom interactions with high resolution LEED/Auger to examine long- and short-range order of chemisorbed layers. Monte Carlo simulations and transfer-matrix-scaling calculations of phase diagrams to obtain interaction parameters. Experimental determination of critical exponents associated with two-dimensional phase transitions and comparison with phase transition theory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, MA 02139

382. GRAIN BOUNDARIES

R. W. Balluffi
Dept. of Materials Science and Engineering
Phone: (617) 253-3349
P. D. Bristowe
Dept. of Materials Science and Engineering
Phone: (617) 253-3326

$348,440 01-1

A broad-based, fundamental investigation of the structure and properties of grain boundaries consisting essentially of combined computer simulation and experimental attacks on the problem of determining the atomic structure and corresponding properties of high-angle grain boundaries in metals and ceramic oxides. Materials studied include MgO, Au, Cu, Al, and alloys of Au and Ag. Experimental techniques employed include X-ray diffraction experiments at the NSLS, high-resolution and conventional electron microscopy and computer simulation.

383. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS

W. D. Kingery
Dept. of Materials Science and Engineering
Phone: (617) 253-3319
R. L. Coble
Dept. of Materials Science and Engineering
Phone: (617) 253-3318

$398,938 01-1

Electrical and optical behavior of Al_2O_3 and MgO including vacuum ultraviolet spectroscopy characterization of band gaps. Float zone laser crystal growth and zone refining in Al_2O_3. Grain boundary migration in high purity powder and bicrystals of Al_2O_3. Kinetic studies include oxygen diffusion measurements in MgO by gas exchange and SIMS, reaction processes and microstructure development in low-temperature sub-solidus systems, rapid quenching effects in a eutectic Ca-Mg-silicate liquid phase and the Fe-Cu two phase system, suppression of insulator charging in SEM and SIMS measurements, grain boundary diffusion in $SrTiO_3$, and Bi and O grain boundary diffusion in ZnO. Defect structures, defect interaction, grain boundary and surface studies including point defects in SiC, B, and C distribution in doped SiC, grain boundary microchemistry and slow crack growth in SiC, influence of microstructure and grain boundary segregation on electrical properties of polycrystalline ZnO, grain boundary segregation in polycrystalline Al_2O_3, segregation at special grain boundaries in MgO, influence at grain boundary composition on grain boundary diffusion, structure of a migrating low angle tilt grain boundary in $SrTiO_3$, and role of grain boundary segregation on high temperature deformation in SiC and Al_2O_3. Sintering studies include atom transport, processing and sintering of SiC, grain boundary mobility in alkali halides, test of the applicability of Herring's scaling law, the effect of MgO on sintering of Al_2O_3, and orientation effects on the grain boundary migration of high purity Al_2O_3.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

384. MECHANISMS OF TRANSFORMATION TOUGHENING

G. B. Olson
Dept. of Materials Science and Engineering
Phone: (617) 253-6901
I.-W. Chen
Dept. of Materials Science and Engineering
Phone: (617) 253-6901
D. M. Parks
Dept. of Materials Science and Engineering
Phone: (617) 253-6901

$188,745 01-2

Constitutive relations experimentally determined for various homogeneous and composite systems. The flow laws developed used to model macroscopic ductility and local plasticity at cracks and interfaces. Model materials selected for study include austenitic and martensitic steels, composites of oxide particles dispersed in metallic and in silicate-glass matrices, composites of alkali-halide particles in ceramics, and amorphous metals.

385. RAPIDLY SOLIDIFIED CERAMICS: PROCESSING, STRUCTURE, AND MAGNETIC PROPERTIES

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

$115,498 01-3

Rapid solidification studies of the systems Al_2O_3-ZrO_2, Al_2O_3-MgO, Y_2O_3-ZrO_2, selected ternary compositions from the previous binary systems, Ba ferrite, and Ni-Zn ferrite. Sample preparation by means of a 1500 watt CO_2 laser to melt feed rods of the desired composition, melt spinning, a 1000 watt CO_2 laser to perform surface melting and regrowth experiments at controlled solid-liquid interface velocities, and ultrasonic atomization. Sample characterization by means of STEM, XRD, EXAFS, IR and Raman spectroscopy, vibrating sample magnetometry and B-H hysteresis loops and magnetic permeability for soft ferrites.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

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

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

$100,000 01-3

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

387. MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS

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

$182,000 01-3

This research project is investigating the mechanisms of oxidation and oxidation/sulfidation of metals at elevated temperatures. Emphasis will be placed on behavior of alloys that form protective refractory oxide scales such as Cr_2O_3 and Al_2O_3 during oxidation and on factors controlling scale degradation in gas mixture having a high sulfur to oxygen activity. In addition, the influence of very fine-grained microstructures (rapidly solidified materials) of the substrate on mechanisms of oxide formation and breakdown in gas mixtures will be examined.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

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

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

$154,270 01-4

Fundamental research to characterize the irradiation stability and radiation damage microstructures of crystalline ceramic solids with application to nuclear energy production and disposal of high-level nuclear waste. The principal mode of investigation is transmission electron microscopy. Materials to be examined include BeO, $MgO \cdot nAl_2O_3$, CaF_2, PuO_2, ZrO_2, SiC, Si_3N_4, Li_2O, $LiAlO_2$, $LiAl_5O_8$, Li_2ZrO_3, $Ca(Zr,Pu)Ti_2O_7$, titanate pyrochlores, SiO, GeO, $ZrSiO_4$. Neutron, ion and electron irradiation damage will be studied, including the effects of massive -recoil nuclei and fission fragments.

389. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

H. K. Bowen
Dept. of Materials Science and Engineering
Phone: (617) 253-6892

$125,015 (17 months) 01-5

Development of a scientific basis for the processing and packing behavior of the model sub-micron ceramic powders SiO_2, TiO_2, and SiC. Synthesis aspects of the colloid chemistry and mono-sized particle masses. Colloid coagulation. Surface chemistry and powder characterization. Ordering behavior of particulate assemblies. Effects of particle size distribution on slurry stability. Dispersion, packing, and sintering behavior. Generalizations controlling the presintered structure of compacts containing 10^{12} particles. Laser diffraction. Photon correlation spectroscopy.

390. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

C. G. Shull
Dept. of Physics
Phone: (617) 253-4812

$156,607 02-1

Investigation of the fundamental properties of neutrons and their interactions with crystalline solids. Establishment of an upper limit on the magnetic neutrality of the neutron. Study of the dynamical theory of neutron diffraction and its consequences: Pendellosing phenomena and Larmor precession effects on neutrons passing through crystalline matter.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

391. SUBMICRON LAYERS OF Nb-Al

S. Foner
Francis Bitter National Magnet Laboratory
Phone: (617) 352-5572

$112,500 02-2

Basic studies of the properties of layered structures as prototypical systems of low temperature reacted niobium-aluminum. Bilayers and multilayers of Nb and Al employed to investigate the effects on the physical properties of structure, composition and content of oxygen and other additives. Study of proximity effects and mechanisms for high critical current in thin layers. Methods of achieving optimum atomic order in these structures will be sought. Research on the applicability of these studies to a wider class of other promising high critical current, field and temperature Nb_3X compounds.

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

R. H. Meservey
Francis Bitter National Magnet Laboratory
Phone: (617) 253-5578
P. M. Tedrow
Francis Bitter National Magnet Laboratory
Phone: (617) 253-0281

$143,750 02-2

The A15 compound V_3Ga is the best known superconducting material for the fabrication of practical high field magnets, restricted however, to critical magnetic fields of about 25T. It is believed that this restriction is due to Pauli paramagnetism in the presence of weak spin-orbit (SO) scattering by the low-Z elemental components, and that it can be eased by increasing the SO scattering rate -- which is believed to scale with the fourth power of the atomic number Z. Two approaches to increasing the SO scattering rate: inclusion of high-Z impurities placed randomly but with minimal introduction of lattice disorder, and inclusion of thin closely spaced layers of high-Z materials. Samples prepared by electron beam evaporation and characterized by superconducting properties, resistivity, and spin-polarized tunneling measurements. Aim to test existing theoretical concepts, to advance understanding of high field superconductors and of many-body effects in normal transition metal systems, to develop improved magnetic solenoids.

MIAMI UNIVERSITY
Oxford, OH 45056

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

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

$55,000 02-2

Investigation of magnetic multilayers (MoNi and VNi) using ferromagnetic resonance. Measurement of the frequency dependence of the anisotropy, and spectral lineshapes. Collaboration will fabricate and characterize the magnetic multilayer samples.

MICHIGAN STATE UNIVERSITY
East Lansing, MI 48824

394. DYNAMIC RECRYSTALLIZATION DURING HIGH-TEMPERATURE LOW-CYCLE FATIGUE OF NICKEL

G. Gottstein
Dept. of Metallurgy, Mechanics, and Materials Science
Phone: (517) 353-5103

$70,981 01-2

Investigation to establish the conditions, limits, and criteria for the occurrence of dynamic recrystallization and its impact on materials performance during low cycle fatigue of Ni and Ni_3Al. Analysis of dislocation structure, subboundary misorientation and internal stresses at subboundary joints. Correlation of dislocation substructure and dynamic recovery kinetics with nucleation of dynamic recrystallization. Dependence and impact of dynamic recrystallization on strain localization, crack nucleation, and crack growth. Development and control of dynamically recrystallized structure, grain size and texture. Characterization techniques include mechanical testing, TEM, and STEM, X-ray pole figure measurements and X-ray micro-Laue diffraction.

MICHIGAN TECHNOLOGICAL UNIVERSITY
Houghton, MI 49931

395. STRESS CORROSION CRACKING AND METAL INDUCED EMBRITTLEMENT: COMPARATIVE STUDIES OF LOCAL CHEMISTRY AND KINETICS

L. A. Heldt
Dept. of Metallurgical Eng.
Phone: (906) 487-2630
M. B. Hintz
Dept. of Metallurgical Eng.
Phone: (906) 487-2630

$93,000 01-2

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

396. THEORY OF DEFECTS IN NON-METALLIC SOLIDS

A. B. Kunz
Dept. of Physics and Institute of Condensed Matter Studies
Phone: (906) 487-2277

$99,000 (16 months) 02-3

Calculations for impurities in oxides combining fully self-consistent correlated electronic structure calculations with shell model calculations of host polarization and distortion. The electric structure and lattice relaxation components are integrated self-consistently to obtain absolute energies of impurity ions in their several charge states in a given host and to obtain interatomic interactions suitable for a broad range of calculations. Emphasis on cases for quantum mechanical treatment where conventional empirical methods are inadequate. Calculations cover various defect and impurity centers, mainly in oxide crystals, including transition metal ions, anion defects, and H and C, in each case several charge states will be considered.

UNIVERSITY OF MICHIGAN
Ann Arbor, MI 48109

397. EFFECT OF MICROSTRUCTURE ON THE MECHANICAL PROPERTIES OF SILICON NITRIDE CERAMICS

T. Y. Tien
Dept. of Materials & Metallurgical Engineering
Phone: (313) 764-9449

$101,133 01-1

Study the role and mechanism of nucleating agents on the crystallization of the Si_2N_2O containing boundary phases which are formed during the processing of Si_3N_4 (containing Y_2O_3 and Al_2O_3) and SIALON ceramics including SIALON-Cordierite. Microstructure and phase identification in sintered and hot pressed specimens. X-ray diffraction, scanning transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

398. THE INFLUENCE OF GRAIN BOUNDARY CHEMISTRY AND STRUCTURE ON THE INTERGRANULAR ATTACK AND INTERGRANULAR STRESS CORROSION CRACKING OF AUSTENITIC ALLOYS

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

$134,253 01-2

The proposed program will focus on SCC in tetrathionate solutions, in NaOH at 140^{o}C and in high temperature high purity water. Tests will be performed on alloys heat treated to produce various degrees of grain boundary chromium depletion along with impurity segregation. Molecular dynamics and molecular orbital calculations will be performed to assess the influence of hydrogen in combination with grain boundary segregants on embrittlement. Tests will be performed to quantify the degree of embrittlement. Work on the quantitative determination of P segregation to the grain boundary will be continued, and the effects of B and N addition on carbide morphology, nucleation, growth, and Cr diffusion will be studied.

UNIVERSITY OF MICHIGAN (continued)

399. INVESTIGATIONS ON THE MBE GROWTH AND PROPERTIES OF AlGaInAs/InP AND InGaAs-InAlAs SUPERLATTICES

P. K. Bhattacharya
Dept. of Electrical Engineering and Computer Science
Phone: (313) 763-6678
A. Brown
Dept. of Electrical Engineering and Computer Science
Phone: (313) 763-3350
R. Gibala
Dept. of Materials and Metallurgical Engineering
Phone: (313) 763-4970

$125,060 01-3

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

400. GROWTH AND DYNAMICS OF SCALE INVARIANT MATTER

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

$155,000 02-3

Theory of the growth, morphology and dynamics of systems having significant scale-invariant fractal-like structures. Such structures have been found to occur over a broad range of materials, for example, in smoke, colloids, deposition of electrolytes, and percolation clusters. Both analytical techniques and numerical simulations are applied. Primary concentration on (1) what properties of growth process determine universality classes, (2) relation of non-equilibrium to equilibrium growth processes, (3) systematic description of growth and reliable calculation of large-scale structures, (4) dynamics on fully developed structures, e.g. diffusion and statistical behavior.

UNIVERSITY OF MINNESOTA
Minneapolis, MN 55455

401. CORROSION RESEARCH CENTER

R. A. Oriani
Dept. of Chemical Engineering and Materials Science
Phone: (612) 373-4864
D. A. Shores
Dept. of Chemical Engineering and Materials Science
Phone: (612) 373-4183
W. H. Smyrl
Dept. of Chemical Engineering and Materials Science
Phone: (612) 373-2763

$840,579 01-1

Interactive fundamental research in two areas: high temperature corrosion and aqueous corrosion. Emphasis in the former area on characterizing the development of stresses and cracks in oxide scales formed on metals and ceramics as well as on identifying the role of processes other than bulk diffusion in complex scales exposed to corrosive gaseous and molten salt environments. Aqueous corrosion research includes both modeling and experimental efforts in the evaluation of corrosion in systems where protective films do not form as well as in those where passive films control corrosion.

402. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS

W. W. Gerberich
Dept. of Chemical Engineering and Materials Science
Phone: (612) 373-4829

$83,827 01-2

Time- and temperature-dependent effects on fatigue threshold in polycrystalline metals. Investigation of influence of closure as well as internal resistance on crack advance in Fe-Si single- and polycrystalline materials. Intrinsic variables: frequency and temperature dependence, dislocation substructure. Extrinsic variables affecting closure: dwell-time and mean stress. Load ratio effects on cyclic cleavage with and without hydrogen. Novel techniques: acoustic emission in conjunction with programmed mechanical loading to understand discontinuous cracking; electron channeling to analyze near-surface deformation.

UNIVERSITY OF MINNESOTA (continued)

403. VERY LOW TEMPERATURE STUDIES OF HYPERFINE EFFECTS IN METALS

W. Weyhmann
School of Physics and Astronomy
Phone: (612) 373-5481

$104,705 (15 months) 02-2

Studies of magnetic interactions in metallic systems using nuclei as probes of the hyperfine fields with emphasis on the role of electrons. Investigations of three types of materials: nuclear singlet ground state intermetallic compounds, very dilute magnetic impurities in non-magnetic metals, and itinerant ferromagnets. Development of the sub-millikelvin capabilities of the first type and utilization of these capabilities to study local moments in manganese-based Kondo systems at very low temperatures. Local magnetization studies using nuclear orientation and macroscopic magnetization measurements using SQUID magnetometry. Search for electron polarization effects in itinerant ferromagnets using nuclear orientation.

UNIVERSITY OF MISSOURI/COLUMBIA
Columbia, MO 65211

404. PHOTOCONDUCTIVITY AND EMISSION FROM THE IMPURITY EXCITED STATES IN SILICON

H. R. Chandrasekhar
Dept. of Physics & Astronomy
Phone: (314) 882-6086

$55,947 02-2

Investigation of excited states in silicon via selective population of these states by tunable laser excitation while simultaneously probing sample materials by means of photoconductivity or emission spectroscopy. Excitation and recombination rates measured and used in identifying the impurity excited states. Effects due to resonant interactions between localized phonons and the impurity states or the electronic continuum also studied. Expect to establish the feasibility of a new type of extrinsic detector of infrared in the 200-100 m range.

UNIVERSITY OF MISSOURI/COLUMBIA (continued)

405. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION

W. B. Yelon
Dept. of Physics
Phone: (314) 882-4211
G. Schupp
Dept. of Physics
Phone: (314) 882-4211

$80,557 02-2

A variety of condensed matter experiments using the 46.5 keV Mossbauer transition in tungsten-183 produced at the Missouri University Research Reactor, which is a thousand times more intense than conventional Mossbauer sources. Quasi-elastic scattering in a liquid metal study of self-diffusion as a function of temperature; Elastic-inelastic separation of the diffracted radiation in zinc to study large anomalous anharmonic contributions to the scattering; A determination of the charge density wave satellites in TaS_2 near the commensurate-incommensurate first order phase transition. An improved measurement of the asymmetry parameter of the 46.5 keV transition. Experiments to separate the elastic and inelastic scattering at Bragg reflections for measurement of the quasi-elastic linewidths near critical points. Signal to noise for these experiments enhanced through the use of a specially developed microscopic conversion electron (MICE) detector: additional isotopes will be tried. In collaboration with J. G. Mullen at Purdue.

UNIVERSITY OF MISSOURI/KANSAS CITY
1110 E. 48th Street
Kansas City, MO 64110

406. THEORETICAL STUDIES ON THE STRUCTURES OF INSULATING AND METALLIC GLASSES

W-Y. Ching
Dept. of Physics
Phone: (816) 276-1604

$76,472 01-1

Theoretical study of atomic scale, electronic, and dynamic structures of insulating and metallic glasses. Construction of structure models for various noncrystalline solids with periodic boundary conditions. First-principles quantum mechanical calculations of electronic states and vibrational spectra, with emphasis on microscopic information on the localization of electron states and their correlations to the short-range order of the model structure. Approach is to perform exact microscopic OLCAO calculations for the eigenvalues and eigenvectors for model Hamiltonians corresponding to model structures with one to two hundred atoms and periodic boundary conditions.

UNIVERSITY OF MISSOURI/ROLLA
Rolla, MO 65401

407. CHARACTERIZATION OF THE REDOX BEHAVIOR AND STABILITY OF ELECTRICALLY CONDUCTING OXIDES

H. U. Anderson
Dept. of Ceramic Engineering
Phone: (314) 341-4886

$119,288 01-3

Interrelationships between electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n- and p-type binary and ternary transition metal oxides. 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. Experiments include specimen preparation, thermogravimetric characterization, optical microscopy, X-ray diffraction, TEM, electrical conductivity, EPR, thermally stimulated current, optical absorption, and oxygen diffusion.

UNIVERSITY OF NEBRASKA
Lincoln, NE 68588-0111

408. MAGNETIC STUDIES OF IRON:RARE-EARTH:METALLOID ALLOYS

D. J. Sellmyer
Dept. of Physics
Phone: (402) 472-2407

$ 51,560 02-2

Investigation of the new iron:rare-earth:metalloid alloys with high potential for permanent magnetic applications including $Fe_{77}R_{15}M_8$ and $Fe_{82}R_{12}M_6$ where R is primarily a rare-earth and M is a metalloid such as B, C, and Si. Main emphasis on preparation techniques, correlation of magnetic properties of 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

409. ENERGY TRANSFER BY TRIPLET EXCITON MIGRATION IN POLYMERIC SYSTEMS

R. D. Burkhart
Dept. of Chemistry
Phone: (702) 784-6041

$90,000 03-1

Studies of triplet-triplet annihilation and rate of triplet exciton diffusion in polymers. Direct excitation of ground state polymer chromophores to lowest triplet state through dye laser pumping. Investigation of the rate of triplet exciton migration in polymers having pendant groups which are sterically crowded and non-planar to asses the extent to which structural modifications can influence rates of exciton migration.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 97131

410. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE COMPLEX Nb-Ta-Ti OXIDES, PHOSPHATES, AND SILICATES

R. C. Ewing
Dept. of Geology
Phone: (415) 277-4163

$75,902 01-1

Comparative study of the properties of selected metamict minerals and synthetic irradiated phases of similar compositions. Research includes characterization of changes in properties of crystalline materials as a function of an alpha-recoil dose for natural materials; characterization of the structure of the metamict state in various silicates, phosphates, and oxides using X-ray diffraction, electron microscopy, extended X-ray absorption fine structure and near edge structure (EXAFS/XANES) spectroscopy; determination of kinetics of annealing of natural zircons, pyrochlores and silicate apatites, and complex Nb-Ta-Ti oxides which are partially or completely metamict; and correlation of recrystallization and fission track fading kinetics to predict the role of thermal annealing on long-term radiation effects.

UNIVERSITY OF NEW MEXICO (continued)

411. ICOSAHEDRAL BORON-RICH SOLIDS AS VERY-HIGH TEMPERATURE THERMOELECTRICS AND SEMICONDUCTORS

C. L. Beckel
Dept. of Physics
Phone: (505) 277-2449
V. M. Kenkre
Dept. of Physics
Phone: (505) 277-2616
D. Emin
Dept. of Physics
Phone: (505) 277-8602

$176,000 (2 years) 02-3

Theoretical studies of boron-rich solids with structures typically consisting of boron icosahedra strongly linked by two or three atom chains, and stable to very high temperatures. Examples: pure and doped $B_{12}C_2$, $B_{12}P_2$, $B_{12}As_2$, and other compositions such as B_4C. Focus on test of theoretical models through prediction of electronic, vibrational, heat transfer and optical properties. Collective expertise of four person theoretical team directed toward understanding and controlling these properties at a microscopic level. Polaron theory, cluster-based electronic calculation, classical force field calculations, transport of electronic and vibrational excitation by diffusion of extended excitations and/or by hopping of localized excitations. Soluble models of primary physical mechanisms. Quantitative theoretical descriptions, but generally not ab initio computation (due to complexity of the systems), with self-consistency both in electronic structure and of equilibrium geometry. Significant technological as well as scientific interest, primarily in potential use of borides in very-high temperature semiconductor and/or thermoelectric applications. Theoretical effort strongly interactive with a major experimental program involving SNL/A, JPL, and UNM.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE
New York, NY 10031

412. INVESTIGATIONS OF HARD, CARBON-BASED SURFACE COATINGS: FROM "DIAMOND-LIKE" CARBON TO SILICON CARBIDE

F. W. Smith
Dept. of Physics
Phone: (212) 690-6963

$105,657 01-1

Preparation of thin-film surface coatings by glow discharge and reactive sputtering of disordered alloys of carbon, silicon, and hydrogen ($C_xSi_yH_z$) with carbon as the primary constituent. Characterization using photoemission, EXAFS, optical spectroscopy (visible and IR) and measurements of density and hardness. Photoemission and carbon K-edge absorption studies using synchrotron radiation at the BNL NSLS.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

413. DYNAMICS OF FLUID SURFACES AND THE CRYSTAL-MELT INTERFACE

H. Z. Cummins
Dept. of Physics
Phone: (212) 690-6921

$112,704 02-2

Study by quasielastic light scattering spectroscopy of two closely related phenomena associated with interfacial dynamics: capillary waves on the free surface of a liquid as a function of temperature, and of the microscopic dynamics of growth - accomplished by investigating the nature of excitations on the interface of a crystal growing into an undercooled melt. To elucidate various aspects of the surface roughening transitions, the genesis of screw dislocations and ultimately, the morphological instability of a growing crystal surface for dendrite formation.

414. MAGNETIC PROPERTIES OF DOPED SEMICONDUCTORS

M. Sarachik
Dept. of Physics
Phone: (212) 690-8206

$100,000 02-2

A precise systematic study of the magnetic properties of homogeneous, well-characterized samples of heavily doped semiconductors as a function of impurity concentration across the metal-nonmetal transition. Faraday balance measurements as a function of temperature (from 1.25 K to 300 K) and of magnetic field (to 50 kG) to separate various contributions to the total susceptibility. The measurements will be extended to 50 mK and 190 kG at the National Magnet Laboratory. The role percolation has in the transition will be determined.

415. CONDUCTION AND PROPAGATION IN DISORDERED SYSTEMS

M. Lax
Dept. of Physics
Phone: (212) 690-6864, (201) 582-6527

$113,153 02-3

Theoretical research concerned, in part, with hopping conductivity in multi-dimensional systems, including quasi-one-dimensional organic chains such as polyacetylene, and even DNA. Work on the production, propagation, screening and isotope scattering of terahertz phonons in GaAs. Application of multiple scattering techniques to scattering from random, wavy surfaces. Emphasis on transport in small systems whose size can be comparable to the mean free path.

CITY UNIVERSITY OF NEW YORK/QUEENS COLLEGE
Flushing, NY 11367

416. DIRECT SYNTHESIS AND OPTIMIZATION OF Fe-BASED, RARE-EARTH, TRANSITION METAL PERMANENT MAGNET SYSTEMS

F. J. Cadieu
Dept. of Physics
Phone: (718) 520-7463

$164,690 01-1

Prepare and characterize polycomponent metal films of $Nd_2Fe_{14}B$, and related $R_2Fe_{14}B$ systems, $(Sm + Ti)Fe_5$, $Sm(Ti,Fe)_2$ and $Sm_2(Co,Fe,Zr)_{17}$ under a variety of conditions by RF sputtering. Films made with and without a composition gradient along the length of the substrates. Selectively thermalized sputtering employed to yield highly textured and metastable structures to aid in the direct growth of crystallographically orientated samples. X-ray diffraction, X-ray fluorescence analysis and electron microprobe will be employed to determine crystal structure and composition variations. High field magnetization and electron energy loss spectroscopy measurements on films with varying crystallographic texturing-selected magneto-optical measurements will be carried out.

POLYTECHNIC INSTITUTE OF NEW YORK
333 Jay Street
Brooklyn, NY 11201

417. MIXED VALENT BEHAVIOR IN ACTINIDES AND RELATIONSHIP TO CERIUM

P. S. Riseborough
Dept. of Physics
Phone: (212) 643-5011

$75,550 02-3

Theoretical research on the manybody aspects of materials containing the early actinide elements and cerium. Principal subject areas: the direct relationships between the magnetic properties, conduction electron-spin scattering effects in transport properties, and the single particle excitation spectrum (as seen in photoemission and Bremsstrahlung Isochromat spectroscopies). Basic theoretical model: a lattice of magnetic ions (the Anderson Lattice) in which the magnetic f-electrons can be delocalized by both the direct f-f overlap and the hybridization with the valence band. Also a study of electron phonon-mediated couplings and other possible exotic coupling mechanisms in the heavy fermion superconductors $CeCu_2Si_2$, UBe_3, and UPt_3.

STATE UNIVERSITY OF NEW YORK/BUFFALO
BUFFALO, NY 14214

418. CONSTRUCTION AND OPERATIONS OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

P. Coppens
Dept. of Chemistry
Phone: (716) 831-3911

$400,000 02-2

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/STONY BROOK
Stony Brook, NY 11794

419. INTERFACE PROPERTIES AND CRYSTAL-GROWTH MECHANISMS

J. Q. Broughton
Dept. of Materials Science and Engineering
Phone: (516) 632-8492, 8493, 8484

$69,861 01-1

Use of computer simulation methods to examine synergistic effects of roughening and surface melting in crystal-vapor systems; mechanism of impurity incorporation in rapidly growing crystals; anisotropy of growth velocity with different crystal faces in crystal-melt systems; incidence of melt regions forming in grain boundaries at high temperatures; rough-smooth transitions observed in MBE grown crystal-vapor systems; influence of directional bonding (e.g., in network formers like Si) on interface width, growth, velocity, impurity trapping, and roughening temperature.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

420. RESEARCH CONSORTIUM FOR X-RAY TOPOGRAPHY ON LINE X-19 AT NSLS

A. H. King
Dept. of Materials Science
Phone: (516) 246-6786
M. Dudley
Dept. of Materials Science
Phone: (516) 246-6778

$481,000 01-1

Implementation of facilities and research for the Synchrotron Topography Project beamline X-19C at the National Synchrotron Light Source at Brookhaven National Laboratory under the auspices of a National Consortium headed by the SUNY Stony Brook group. The consortium is continuing work on a wide range of problems where the special properties of synchrotron radiation are particularly suited including: studies of the factors controlling elastic-plastic crack propagation, real-time slip initiation observations, quality assessment of crystal growth, mechanical integrity of thin film-substrate interfaces, thermal decomposition mechanisms for inorganic single crystals, in situ measurements of the film stresses accompanying film deposition for refractory metal silicides on silicon, detailed studies of the interaction of acoustic waves with microstructural constituents, morphology of pressure quenched CdS and X-ray topography and microradiography aimed at understanding high temperature deformation mechanisms of steels.

The members of the Participating Research Team (PRT) for X-ray topography include Professor J. Bilello (Project Director), Professor H. Chen (Univ. of Illinois), Professor R. Green (Johns Hopkins Univ.), Professors P. Herley and H. Herman (Stony Brook), Professor D. Pope (Univ. of Pennsylvania), Professor R. MacCrone (RPI), Drs. M. Suenaga, J. Hastings, and W. Thomlinson (BNL), and Dr. J. Patel (Bell Labs, Murray Hill). Associated Users include Drs. D. Davidson (SRI), S. Stock (Northwestern Univ.), and S. Weissman (Rutgers Univ.).

421. SURFACE STUDIES BY A VUV PRT AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

F. Jona
Dept. of Materials Science and Engineering
Phone: (516) 246-7649, 6759

$161,439 02-2

Development of versatile ultrahigh vacuum experimental apparatus for surface research with the VUV ring, beam line U7, at the National Synchrotron Light Source (NSLS) incorporating LEED, AES, SEXAFS, and photoemission facilities. Studies of electron core level shifts and valence band configuration changes in alloys relative to pure metals and of single crystal surfaces. Angle-integrated and angle-resolved measurement, development of recently demonstrated resonant photoemission capabilities, adatom locations and characteristics.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

422. KINETICS OF PHASE SEPARATION IN POLYMER SOLUTIONS

B. Chu
Dept. of Chemistry
Phone: (516) 246-7792

$85,000 03-1

Kinetics of phase separation in polymer solutions and blends. Structure of phase separated droplets. Size, shape, and distribution of micro domains measured using light and X-ray scattering, excimer fluorescence, 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.

423. THEORETICAL STUDIES OF CHEMIADSORPTION ON COPPER-NICKEL ALLOYS AND SURFACE EMBRITTLEMENT

J. L. Whitten
Dept. of Chemistry
Phone: (516) 246-6068

$100,000 03-3

Theoretical study of the structure and energetics of molecules adsorbed on solid surfaces and dissociative chemiadsorption with emphasis on transition metal substrates. Systems studied are titanium, copper, nickel and copper/nickel substrates, and H_2, H, CO, C and coabsorbed H and C adsorbates. Emphasis is on the energetics of adsorption as a function of surface site and composition to determine the reactivity of adsorbed species. Theory focuses on an accurate, _ab initio_ treatment of the localized and delocalized interactions that occur in the case of adsorption on metals with active d electrons.

NEW YORK UNIVERSITY
4 Washington Place
New York, NY 10003

424. PHOTOEMISSION STUDIES OF F-ELECTRON SYSTEMS: MANY BODY EFFECTS

S. J. Williamson
Dept. of Physics
Phone: (212) 598-2867

$100,000 02-2

Photoemission studies of f-electron behavior in metallic rare earth and early actinide systems. Electronic phenomena associated with mixed valent and Kondo lattice systems, hybridization effects between f-electrons and either near neighbor ligands or conduction electrons and itinerant versus localized behavior of f-electrons in expanded uranium-based systems. Techniques employed include deep core XPS, ultra-high resolution UV-stimulated photoemission and synchrotron light-stimulated photoemission.

NORTH CAROLINA AGRICULTURAL & TECH. UNIV
Greensboro, NC 27411

425. EFFECT OF THERMAL AND CYCLIC LOADS ON SILICON CARBIDE YARN REINFORCED GLASS MATRIX COMPOSITES

V. S. Avva
Dept. of Mechanical Engineering
Phone: (919) 379-7620
J. Sankar
Dept. of Mechanical Engineering
Phone: (919) 379-7620

$67,340 01-5

Characterization of SiC/glass matrix fibers before, during, and after tension-tension and thermal fatigue testing from room temperature to 600°C at a stress amplitude ratio of 0.1 and a frequency of 10Hz. Radiographic examination for delaminations, debonding, fiber breakage, etc. Optical and scanning electron microscopy microstructural characterization.

NORTH CAROLINA CENTRAL UNIVERSITY
Durum, NC 27707

426. VIBRATIONAL PROPERTIES OF DISORDERED SOLIDS: FAR INFRARED STUDIES

J. M. Dutta
Dept. of Physics
Phone: (919) 683-6452
C. R. Jones
Dept. of Physics
Phone: (919) 683-6452

$86,903 (15 months) 02-2

Measurements of low-frequency vibrational properties of disordered solids in the far infrared region (5 cm^{-1} to 150 cm^{-1}) as a function of temperature using laser techniques. Materials studied: various forms of quartz and fused silica, alumina and magnesia. Other materials of interest: BeO, BN, and Si_3N_4. Effects on dielectric properties due to the presence and concentration of impurities and sintering acids, and to microstructural properties, investigated in selected materials. Experimental data compared with existing theoretical models.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27695

427. MICROSTRUCTURAL EFFECTS IN SOLID PARTICLE EROSION

R. O. Scattergood
Dept. of Materials Engineering
Phone: (919) 737-7843
H. Conrad
Dept. of Materials Engineering
Phone: (919) 737-7843

$91,153 01-5

Correlation of erosion rates in multiphase systems with constituent phase properties and distribution. Systems under investigation: Al-Si alloys, WC-Co cermets, SiC-reinforced alumina and alumina-stainless steel composites, and sintered alumina. Systematic measurement of erosion rates as a function of operational variables (particle size, velocity, angle-of-incidence) and microstructural variables (volume fraction, phase size and distribution, alloy content). SEM observations on steady-state erosion surfaces and single impact events. Constitutive and averaging laws for erosion rates to be developed from experimental results and modeling/ computer simulation.

NORTH CAROLINA STATE UNIVERSITY (continued)

428. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR PRT STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY

D. E. Sayers
Dept. of Physics
Phone: (919) 737-2512

$315,000 02-2

Development of an advanced soft X-ray Absorption Spectroscopy and Extended X-ray Absorption Fine Structure (EXAFS) beam line at the National Synchrotron Light Source for a Participating Research Team (PRT) with active members from North Carolina State University, Universities of Connecticut and Washington, Brookhaven and Argonne National Laboratories, General Electric, Mobil, and Dupont. Facilities for EXAFS, fluorescence, near-edge absorption, and polarization studies from about 1 to 20 keV. Research in amorphous alloys, surface layers, catalysis, gases adsorbed in metals, magnetic and time-dependent phenomena, electrochemistry, and technique development.

429. BAND ELECTRONIC STRUCTURES AND CRYSTAL PACKING FORCES OF ET SALTS

M. H. Whangbo
Department of Chemistry
Phone: (919) 737-3616

$105,000 03-1

Theoretical studies of superconducting and conducting, organic charge transfer salts. Tight-binding band electronic structure calculations on bis(ethylenedithio)tetrathiafulvalene (ET) salts using extended Huckel method. SCF-MO calculations on neutral and charged ET. Calculation of crystal packing energies, stabilities of different crystal phases, and magnitudes of electron-phonon coupling constants of various ET salts.

NORTHEASTERN UNIVERSITY
Boston, MA 02115

430. POSITRON STUDIES OF DEFECTED METALS AND METALLIC SURFACES

A. Bansil
Dept. of Physics
Phone: (617) 437-2902

$108,000 (16 months) 02-3

A theoretical program for investigating the behavior of positrons in imperfect metallic systems and at metallic surfaces. Appropriate generalizations of the current multiple scattering theory techniques undertaken to develop framework capable of describing a wide range of phenomena on a realistic basis. Systems to be investigated: metal and alloy surfaces, metallic glasses, vacancies and vacancy-impurity complexes, and substitutional alloys. Characteristic features of the annihilation process between the positrons and the electrons delineated. A close collaboration with relevant experimental groups planned.

NORTHWESTERN UNIVERSITY
Evanston, IL 60201

431. ELECTRONIC AND STRUCTURAL PROPERTIES OF SEMICONDUCTOR HETEROJUNCTIONS

Y. W. Chung
Dept. of Materials Science and Engineering
Phone: (312) 491-3112

$45,316 01-1

Comprehensive investigation of -Sn fibers deposited in UHV on single crystal CdTe substrate including the study of quantum size effect using high-resolution electron energy loss spectroscopy and optical absorption, determination of relationship between thermal degradation and interfacial diffusion in heterojunctions, determination of film growth characteristics using a site-specific xenon probe technique, and determination of structural and transformation characteristics using surface XRD at the NSLS and electron reflectivity techniques.

NORTHWESTERN UNIVERSITY (continued)

432. POINT DEFECT CLUSTERS AND ELECTRICAL BEHAVIOR IN TRANSITION METAL OXIDES

J. B. Cohen
Dept. of Materials Science and Engineering
Phone: (312) 491-3665
D. E. Ellis
Dept. of Physics and Astronomy
Phone: (312) 491-3665
T. O. Mason
Dept. of Materials Science and Engineering
Phone: (312) 491-3198

$181,574 01-1

Interdisciplinary study of the first row transition metal monoxides, combining measurements of defect structure and electrical properties with quantum theoretical calculations. These oxides represent a "model" series which, while sharing the average structure of NaCl, exhibit a wide range of stoichiometries, defect structures, and conduction mechanisms. Electrical measurements and conduction mechanism analysis will be extended to MnO and NiO. Valence in the series will be studied via X-ray (synchrotron) and/or pulsed neutron scattering. The self consistent field local density theory will be used to calculate the electronic structure associated with isolated vacancies and defect clusters. An energy band code based on the Linearized Muffin Tin Scheme will be used to calculate band structures, Fermi surfaces, and transport properties to correlate with the experimental studies. Extension of theory will be made to more complex oxides, e.g., Fe_3O_4, $CoAl_2O_4$, and $FeAl_2O_4$.

NORTHWESTERN UNIVERSITY (continued)

433. NUCLEAR MAGNETIC RESONANCE CHARACTERIZATION OF POROUS STRUCTURES: CERAMICS AND SANDSTONES

W. P. Halperin
Physics and Astronomy Department
Phone: (312) 491-3686

$89,629 01-1

Application of nuclear magnetic resonance measurements (spin-lattice relaxation and variable length scale diffusion) using a variable length scale pulsed field gradient method (VLS/PFG) to filler fluid nuclei intruded into the pore space of porous materials to give specific information concerning void space microstructure. Experiments with model materials including leached borosilicate (vycor) glasses and packings of monodisperse glass spheres. Investigations of fractal sandstones to define fractal dimension, minimum and maximum fractal length scales, and random-walk dimension for dynamics confined to a fractal. Non-fractal sandstones also investigated to obtain structural parameters and clarify the distinction between dynamics in fractal and non-fractal geometries. Investigation of pore structure evolution in the early and the intermediate stages of sintering of alumina by NMR methods giving direct information on the pore size distribution, throat size, maximum extent of the pore distribution and the distribution of pore surface-to-volume ratios. Evolution of these parameters studied as a function of heating rate and initial compact conditions. Experiments to help to refine sintering models and define relevant processing parameters for attainment of high density.

434. USE OF ANOMALOUS SMALL ANGLE X-RAY SCATTERING TO INVESTIGATE MICROSTRUCTURAL FEATURES IN COMPLEX ALLOYS

J. R. Weertman
Dept. of Materials Science and Engineering
Phone: (312) 491-5353

$80,848 01-2

Investigation of the use of anomalous small angle X-ray scattering (SAXS) 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 SAXS data to obtain quantitative information about the size and number density of each species. Synchrotron radiation will be used to provide X-rays which can be tuned to the absorption edge of elements in the alloy. Anomalous SAXS 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 to be studied will be the ferritic stainless steel, modified Fe9Cr1Mo, which has already been examined by small angle neutron scattering. The value of anomalous SAXS as a method of NDE will be investigated.

NORTHWESTERN UNIVERSITY (continued)

435. DEFECT STRUCTURE OF SEMICONDUCTING AND INSULATING OXIDES

B. W. Wessels
Dept. of Materials Science and Engineering
Phone: (312) 491-3219

$77,466 01-3

Use of space charge spectroscopy techniques to explore the deep level electronic defect structure and its role in charge transport for several semiconducting and semi-insulating oxide compounds. Single crystalline oxide layers prepared by organometallic chemical vapor deposition. Defect phenomena investigated include mechanisms of deep level defect formation, thermal stability of native point defects, and the electrical and optical characterization of deep level defects in as-grown undoped and doped material. Deep level defects formed by high energy electron and proton irradiation. Isochronal annealing. Experimental point defect characterization includes temperature dependent conductivity and photoluminescence measurements. Specific systems to be examined include ZnO, TiO_2, and $SrTiO_3$.

436. STRUCTURAL AND FAST ION TRANSPORT PROPERTIES OF GLASSY AND AMORPHOUS MATERIALS

D. H. Whitmore
Dept. of Materials Science and Engineering
Phone: (312) 491-3533
P. Georgopoulos
Dept. of Materials Science and Engineering
Phone: (312) 491-3243

$116,000 01-3

Detailed structural and ionic transport studies of fast ion conducting glasses including mixed valence, proton conducting and selenide based glasses and amorphous polyphosphazine polymer complexes. Investigation parameters include temperature, glass composition, and conditions of glass synthesis. Computer simulations of ionic transport in glassy electrolytes. Differential anomalous X-ray scattering, EXAFS, Raman and infrared spectroscopies, complex impedance analysis (of conductivity data) and pulsed field gradient NMR (to obtain ionic diffusivities). Mixed valence glasses synthesized by doping glass network formers with appropriate amounts of transition metal compounds investigated for the chemical diffusion coefficient, solid-state redox reactions accompanying the insertion of electroactive alkali ion species into the mixed valence glass and the electronic transference number as a function of glass composition and temperature.

NORTHWESTERN UNIVERSITY (continued)

437. LOCAL DENSITY THEORY OF HEATS OF FORMATION AND SHORT-RANGE-ORDER PARAMETERS IN SUBSTITUTIONALLY DISORDERED ALLOYS

A. J. Freeman
Dept. of Physics and Astronomy
Phone: (312) 491-3343, 3644
A. Gonis
Dept. of Physics and Astronomy
Phone: (312) 491-3644

$76,956 02-3

Determination of thermodynamic properties and, ultimately, phase diagrams of ordered and substitutionally disordered alloys from all-electron calculations that utilize fully relativistic energy band programs and that take into account lattice structure and statistical fluctuations. Particular emphasis is given to heats of formation, to short-range order parameters, and to polyatomic interaction energies. Recently developed methods based on local density theory, on embedded cluster generalizations of the coherent potential approximation, and on a generalized perturbation method are used to obtain the density of states and total energies. Multi-site potentials obtained are to be used, e.g., in cluster variation method computations to construct alloy phase diagrams for transition metals (and, perhaps, actinides).

438. STUDIES OF THE SHEAR RESPONSE AND STRUCTURE OF MONOMOLECULAR FILMS ON THE SURFACE OF WATER

P. Dutta
Dept. of Physics and Astronomy
Phone: (312) 492-5465
J. B. Ketterson
Dept. of Physics and Astronomy
Phone: (312) 492-5468

$91,302 03-3

Study of the mechanical properties of organic monolayers on the surface of water (Langmuir films). The microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) studied using X-rays and ellipsometry. Studies of the mechanical properties directed toward the shear response, an important but previously neglected structural property. A diffraction technique involving external reflection at the monolayer surface used to determine 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, which may be a liquid crystal phase.

UNIVERSITY OF NOTRE DAME
Notre Dame, IN 46556

439. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR

T. H. Kosel
Dept. of Metallurgical Engineering and Materials Science
Phone: (219) 239-5642

$75,052 01-5

Assessment of mechanisms controlling abrasive wear in multiphase Fe- and Co-base alloys, influence of second phase particle toughness, size and volume fraction, changes in near-surface microstructure during abrasion, influence of abrasive size, hardness, angularity and loading conditions, in situ SEM scratch test simulations of fixed-abrasive abrasion mechanisms.

OHIO STATE UNIVERSITY
Columbus, OH 43210

440. INFLUENCE OF NITROGEN ON THE SENSITIZATION, CORROSION, MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF AUSTENITIC STAINLESS STEELS

W. A. T. Clark
Dept. of Metallurgical Engineering
Phone: (614) 422-2538
B. E. Wilde
Dept. of Metallurgical Engineering
Phone: (614) 422-7889

$74,958 01-1

Evaluation of corrosion and stress corrosion cracking of austenitic stainless steel with various carbon and nitrogen contents. TEM characterization of grain boundary structure as well as carbide and nitride morphologies, compositions, and distributions. Measurement of electrochemical parameters in static and flowing aqueous solutions containing chloride and sulphate ions.

441. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

R. A. Rapp
Dept. of Metallurgical Engineering
Phone: (614) 422-6178

$78,867 01-1

In situ SEM study of oxidation of metals, Fe, Ni, Cu and Cr, and binary alloys of these metals, effect of H_2 on oxide morphology, influence of surface treatment on oxidation of Cr, pore development at metal-scale interface, oxide morphologies, e.g., pits and ledges in Fe_2O_3 and whiskers in NiO.

OHIO STATE UNIVERSITY (continued)

442. GENERATION OF MICROPOROSITY IN STEEL WELDS AND ITS ROLE IN HYDROGEN ATTACK

P. G. Shewmon
Dept. of Metallurgical Engineering
Phone: (614) 422-5864

$70,902 01-2

Investigation of mechanisms controlling hydrogen attack in bainitic steels, with emphasis on evaluating degradation in weldments made by various processes--gas tungsten and submerged arc welding as well as electroslag welding, characterization of microporosity with electron microscopy (both TEM and SEM) and dilatometry, respectively, to indicate the microstructural features where attack initiates and the overall kinetics of attack, assessment of role of matrix creep and of susceptibility of fusion vs. heat affected zone to attack.

443. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT BOUNDARIES SEPARATING ANISOTROPIC MATERIALS

L. Adler
Dept. of Welding Engineering
Phone: (614) 422-1974

$107,954 01-5

This is a basic research program on non-destructive characterization of polycrystalline anisotropic materials. Specific activities will include modeling and measurement of ultrasonic wave propagation in bicrystals of Ni and austenitic stainless steel as well as fabrication of specimens and development of techniques.

444. MOLECULAR FERROMAGNETISM

A. J. Epstein
Dept. of Physics
Phone: (614) 422-1133

$120,000 03-1

Study of magnetism in molecular ferromagnets and origins of the ferromagnetic exchange. Synthesis of $[M(C_5(CH_3)_5)_2]^+$ and $[M(C_6R_6)]^+$ (M=Cr, Fe, Ru, and Ni) salts of planar radical anions 7,7,8,8-tetracyano-p-quinodimethane (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- and ferrimagnetism. Mossbauer spectroscopy to measure internal magnetic fields, spectroscopic measurements of charge transfer bands, and inelastic neutron scattering measurements of magnetic structure.

OREGON STATE UNIVERSITY
Corvallis, OR 97331

445. PERTURBED ANGULAR CORRELATIONS IN ZR-CONTAINING CERAMICS

J. A. Gardner
Dept. of Physics
Phone: (503) 754-4631

$58,000 01-1

Perturbed angular correlation (PAC) spectroscopy of nuclear gamma rays to investigate Zr-containing ceramics. PAC characterization of free energies and transformation mechanisms in ZrO_2 based materials. Measurement of ZrO_2 equilibrium phase boundaries and their dependence on purity and stabilizing elements. Analysis of relaxation models and diffusion mechanisms in ZrO_2-Y_2O_3 alloys, short range order and order-disorder reactions, and high-temperature time-dependent effects in various stabilized zirconias. Design and construction of a pressure cell for operation at 200 MPa and 2000°C.

UNIVERSITY OF OREGON
Eugene, OR 97403

446. SURFACE AND INTERFACE ELECTRONIC STRUCTURE

S. D. Kevan
Dept. of Physics
Phone: (503) 686-4742

$143,500 02-2

An experimental investigation of the electronic structure of surfaces and interfaces including studies of angle-resolved photoemission at the National Synchrotron Light Source. Emphasis on high resolution studies of novel surface phenomena such as phase transitions, small perturbations of the ground state electronic structure by defects and impurities, and initial stages of epitaxial interface formation between metals and semiconductors.

447. MONITORING INTERFACIAL DYNAMICS BY PULSED LASER TECHNIQUES

G. L. Richmond
Dept. of Chemistry
Phone: (503) 686-4635

$ 70,125 03-2

Studies of interfacial structure and dynamics using second harmonic generation (SHG) and hyper-Raman scattering. Development of SHG for monitoring electrochemical reactions on a nanosecond and picosecond time-scales, correlation of surface structure and electron-transfer reactivity, thin film nucleation and growth, and analyses of the structure and reactive role of surface defects.

PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

448. PHYSICAL CHEMISTRY OF PORTLAND-CEMENT HYDRATE, RADIOACTIVE-WASTE HOSTS

M. W. Grutzeck
Materials Research Laboratory
Phone: (814) 863-2779

$61,977 01-1

Physical and crystal chemistry of three portland-cement hydrates: calcium silicate hydrates, calcium aluminum hydrates, and calcium alumino silicate hydrates. Phase-equilibrium relationships governing the hydration of portland cement, both with and without radioactive waste. Fixation of iodine by calcium aluminate hydrates and the feasibility of using Stratling's compound and its associated hydrates as host phases for cesium and strontium fixation. Identification of phases best suited for hosting selected radioactive-waste ions, and synthesis and crystallographic characterization of such phases. Solubility/leachability study of synthesized host phases both individually and encapsulated in a suitable cementitious matrix.

449. VIBRATIONAL AND OPTICAL STUDIES OF AMORPHOUS METALS

J. S. Lannin
Dept. of Physics
Phone: (814) 865-9231

$87,792 01-1

Research aimed at developing the method of interference enhanced Raman scattering (IERS) 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.

PENNSYLVANIA STATE UNIVERSITY (continued)

450. SPECTROSCOPIC INVESTIGATIONS OF GLASS STRUCTURE

W. B. White
Materials Research Laboratory
Phone: (814) 865-1152

$43,480 (9 months) 01-1

Glasses containing transition metal ions are studied utilizing Raman, infrared, optical absorption, and luminescence spectroscopy. Specific investigations include (i) the local environment of alkali ions in silicate glasses by far infrared spectroscopy, (ii) processes of phase separations as related to heat treatment by high-temperature Raman spectroscopy, (iii) the relationship of Raman spectra to thermodynamic quantities in silicate glasses, (iv) formation of transition metal complexes in glass, and (v) clustering and nucleation of transition meals in high magnesium content glasses.

451. THE MECHANICAL BEHAVIOR OF SURFACE MODIFIED CERAMICS

D. J. Green
College of Earth and Mineral Sciences
Phone: (814) 863-2011

$98,593 01-2

Modification of surface layers of ceramics to introduce surface compression and increase hardness and fracture toughness of transformation-toughened ZrO_2 and Al_2O_3. Surface infiltration when ceramic is pressed or partially sintered. Development of a second phase surface layer during final densification. Indentation cracking used to study crack nucleation and growth and determine fracture toughness. Stress and composition profiles determined by NSLS X-ray diffraction data.

PENNSYLVANIA STATE UNIVERSITY (continued)

452. TWIN BOUNDARIES AND HETEROPHASE INTERFACES IN FERROELASTIC MARTENSITES

G. R. Barsch
Materials Research Laboratory
Phone: (814) 865-1657

$129,799 01-3

Theoretical study with concurrent supporting experimental investigations on coherent and semicoherent interfaces in ferroelastic martensites, including twin boundaries and twin bands, heterophase parent/product ISP interfaces and inclusions, and transformation precursors. Motivation is the need for a new theoretical basis for investigating the martensite nucleation mechanism and for establishing the conditions for nonclassical nucleation. Study of soliton-like solutions of a dynamic Ginzburg-Landau continuum theory for ferroelastic martensites in order to determine the strain distribution and strain energy for various geometric configurations as a function of the material parameters, temperature and external stress. Model parameters of the theory consist of the second and higher order elastic constants and the harmonic strain gradient coefficients in the parent phase. X-ray measurements of the transformation strain versus temperature, and 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.

453. GRAIN BOUNDARY AND SURFACE DIFFUSION IN OXIDE SYSTEMS

V. S. Stubican
Dept. of Materials Science and Engineering
Phone: (814) 865-9921

$60,808 01-3

This research addresses diffusional transport phenomena on ionic surfaces and grain boundaries. Specifically, studies of surface diffusion of ^{51}Cr on MgO and ^{57}Co on MgO and NiO, and grain boundary diffusion of ^{59}Fe in Fe_3O_4.

PENNSYLVANIA STATE UNIVERSITY (continued)

454. EXPERIMENTAL AND THEORETICAL STUDIES ON TRANSPORT PROCESSES IN LASER WELDING

T. DebRoy
Dept. of Materials Science and Engineering
Phone: (814) 865-1974

$71,326 01-5

Modeling of solute loss, heat transfer and fluid flow during laser welding of stainless steels. Calculation of local temperature profile, weld pool velocity and vaporization of alloying elements, correlative experimental determination of weld microstructure and chemistry, time resolved emission spectroscopic measurements to determine composition of metal vapors.

455. LASER PROCESSING OF CERAMICS

G. L. Messing
Dept. of Materials Science and Engineering
Phone: (814) 865-2262

$63,000 01-5

Correlations between melt crystallization kinetics, thermodynamics, phase equilibria, etc., during rapid solidification of Al_2O_3-SiO_2 compositions around the mullite phase field and Al_2O_3-ZrO_2 both melted with a 10.6 micron CO_2 laser. Preparation of ceramic powders using rapid solidification processing by injecting solutions and/or solid particles coaxially into a plasma flame. Investigation of morphological modification by single particle melting and rapid solidification, calcination of oxide precursors and rapid reaction of multicomponent systems. Formation and properties of mullite powders with respect to phase equilibria, plasma parameters, and solidification conditions.

456. GAS SURFACE INTERACTION USING PULSED-LASER ATOM-PROBE FIELD ION MICROSCOPY

T. T. Tsong
Dept. of Physics
Phone: (814) 865-2813

$68,000 02-2

Experimental investigation of surface catalyzed chemical reactions using pulsed laser time-of-flight atom probe field ion microscopy. Field adsorbed H_3 will be studied on various crystalline surfaces of various metals and alloys. Desorbed ion species such as H^+, D^+, H_2^+, HD^+, D_2^+, H_3^+, H_2D^+, and D_3^+ as a function of tip temperature, tip material, and field strength to determine associative and dissociative mechanisms of hydrogen on various surfaces. Other reactions include methanation of CO and reduction of NO. Adsorption of atoms and molecules on a surface induced by an applied electric field.

PENNSYLVANIA STATE UNIVERSITY (continued)

457. NEW LOW TEMPERATURE (HYDROXYLATED) MATERIALS

R. Roy
Materials Research Laboratory
Phone: (814) 865-3421

$70,200 03-2

Synthesis and characterization of crystalline materials formed at low temperatures. The objective is to apply some of the very new and exciting advances in chemically-bonded ceramics to making much stronger and more impermeable materials that can be processed at low temperatures. The material have potential application as low-level radioactive waste hosts.

UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

458. STAGING IN LAYER INTERCALATES

J. E. Fischer
Dept. of Materials Science and Engineering
Phone: (215) 898-6924

$108,000 01-1

Study of the staging phenomenon in graphite intercalation compounds (principally with Li) and other layer systems by X-ray and neutron diffraction. Independent variables are temperature, hydrostatic pressure and concentration of alkali metal intercalate. Experimental determination of the staging temperature vs. concentration phase diagram. Elucidation of new high-pressure phases. Determination of the nature, origin, and consequences of stage disorder. Investigation of kinetics of staging transitions with emphasis on identifying metastable structures.

UNIVERSITY OF PENNSYLVANIA (continued)

459. ATOMISTIC STUDIES OF THE STRUCTURE AND PROPERTIES OF GRAIN BOUNDARIES WITH SUBSTITUTIONAL IMPURITIES

V. Vitek
Dept. of Materials Science and Engineering
Phone: (215) 898-7883
$24,959 01-1

Atomistic computer simulations to investigate the relationship between the structure of grain boundaries and segregation propensity, the structural changes provoked by the segregation and their effect on boundary behavior, and the transformation of the boundary structures associated with segregation and structural multiplicity. Calculations on segregation propensity for tilt boundaries in iron with Sn, Sb, and Cu as impurities and for twist boundaries in copper with Bi as an impurity. Temperature effects in structural transformations of grain boundaries are investigated by calculating the entropy contributions to the free energy. In addition to the development of semiempirical schemes for describing interatomic forces in the form of pair potentials, a quantum mechanical tight-binding approach to the structural studies of grain boundaries and cohesion at interfaces will be investigated.

460. LOW STRESS BRITTLE FRACTURE IN POLYMERS

N. Brown
Dept. of Materials Science and Engineering
Phone: (215) 898-8506
$98,912 01-2

Initiation of slow crack growth in polyethylene, ethyleneoctene copolymers with various octene concentrations branch densities of 2-10 per 100 carbon atoms and narrow molecular weight distribution. Measurement under plane strain of rate of formation of damaged zone at root of a notch as function of stress, time, temperature, notch depth, specimen geometry. Characterization of extent of porous, fibrillated and fractured regions which constitute the damaged zone using optical microscopy, SEM, and TEM. Determination of constitutive equations for various regions of damaged zone. Use of data to construct a mathematical model based on the micro-mechanics of fracture for predicting long time failure in engineering structures.

UNIVERSITY OF PENNSYLVANIA (continued)

461. FUNDAMENTALS OF HARDENING AND DECOHESION BEHAVIOR IN TIME-DEPENDENT CYCLIC DEFORMATION

C. Laird
Dept. of Materials Science and Engineering
Phone: (215) 898-6664
J. L. Bassani
Dept. of Mech. Eng. and App. Mechs.
Phone: (215) 898-5632

$117,000 01-2

Role of hardening on active and latent slip systems on the deformation of metals under monotonic and cyclic loading; characterization of dislocation structure developed in Cu during time-dependent and time-independent deformation; formulate a physically realistic micromechanical description of the deformation; single crystal behavior followed by polycrystalline materials studies on Cu, Cu-O, and Cu-Pb alloys; cyclic creep deformation and fracture and the role of non-metallic particles on cavity formation and linkage.

462. INTRINSIC SURFACE PHONONS ON RECONSTRUCTED SEMICONDUCTOR SURFACES

E. J. Mele
Dept. of Physics
Phone: (215) 898-3135

$88,745 (17 months) 02-3

Theoretical study of the lattice dynamics of reconstructed semiconductor surfaces. Relation between localized surface electronic and surface structural and vibrational properties. Computation scheme combines a short range elastic Hamiltonian with a static electronic polarization extracted from a tight binding representation of the valence electronic bands. Applications include models of Si(100)2x1 and Si(111)2x1 surfaces and generalization of the results to deduce a structural Hamiltonian for Ge.

UNIVERSITY OF PITTSBURGH
Pittsburgh, PA 15261

463. MICROCHEMISTRY ANALYSIS OF POLYCRYSTALLINE Ni_3Al AND OTHER ORDERED ALLOYS USING THE FIELD-ION MICROSCOPE ATOM PROBE

S. S. Brenner
Dept. of Metallurgical and Materials Engineering
Phone: (412) 624-5445

$115,971 01-1

Investigation of structure and microchemistry of grain boundaries in Ni_3Al containing different Ni/Al stoichiometric ratios, substitutional solutes, and grain boundary B concentrations. Principal analytical methods involve the field-ion microscope atom probe. Other variable parameters include grain-boundary orientation, bulk B concentration, Al substoichiometry, and comparison between cast and melt-spun Ni_3Al-B material.

464. HIGH TEMPERATURE CORROSION OF CERAMICS

F. S. Pettit
Dept. of Metallurgical and Materials Engineering
Phone: (412) 624-5300
J. R. Blachere
Dept. of Metallurgical and Materials Engineering
Phone: (412) 624-5300

$49,999 01-3

Thermodynamic and kinetic analyses of gaseous and molten salt corrosion of oxides (SiO_2, Al_2O_3, Cr_2O_3, and ZrO_2) in oxidizing, sulfudizing, and reducing environments, thermogravimetric measurement of corrosion kinetics. Gas mixtures of SO_2-SO_3-O_2, H_2-H_2O, and CO-CO_2-O_2 at temperatures in the interval 700^o to 1400^oC. Effects of deposits such as Na_2SO_4, NaOH, and Na_2CO_3 on the gas-induced corrosion. Mechanisms of corrosion of high purity materials and of materials with microstructures and impurities characteristic of advanced commercial materials. Morphology of the corrosion products.

UNIVERSITY OF PITTSBURGH (continued)

465. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES

J. V. Maher
Dept. of Physics and Astronomy
Phone: (412) 624-0872

$94,283 02-2

Studies of the physics of binary liquid interfaces. Experiments on onset and nonlinear growth of hydrodynamic instabilities, nonlinear pattern formation, and transition to turbulence. The diffusion-driven instability of a quenched liquid interface and the Saffman-Taylor instability (viscous fingering) investigated with careful control over such parameters as density difference, viscosity difference, and interfacial tension. Light scattering investigations of the dynamics of phase separation for a binary liquid mixture imprisoned in a gel to understand the role of hydrodynamics.

PRINCETON UNIVERSITY
Princeton, NJ 08544

466. THE FORMATION OF ORDERED MICROSTRUCTURES BY SLIP CASTING AND RELATED PROCESSES

W. B. Russel
Dept. of Chemical Engineering
Phone: (609) 452-4590

$70,278 01-3

The dynamics of three processes (sedimentation, ultrafiltration, and slip casting) which concentrate small particles from a dilute solution, with particular emphasis on the structure of the resulting dense phase as a function of the processing conditions. Objectives are to define the range of conditions which produce an ordered casting, develop process models, and perform measurements of diffusion models in dense suspensions. Modeling to involve the formulation and solution of a macroscopic conservation equation governing the mean volume fraction, coupled to a microstructural equation describing the relaxation of imperfections enroute to the equilibrium ordered state. Dynamic light scattering experiments on concentrated silica dispersions to determine diffusion coefficients. Sedimentation and ultrafiltration experiments following the formation of both disordered and ordered phases.

PRINCETON UNIVERSITY (continued)

467. MODULATED INFRARED LINEAR DICHROISM STUDIES OF THE DYNAMICS OF MOLECULAR ORIENTATION AND RELAXATION IN POLYMERS

J. T. Koberstein
Dept. of Chemical Engineering
Phone: (609) 452-5721
R. K. Prud'homme
Dept. of Chemical Engineering
Phone: (609) 452-4577

$84,000 (18 months) 03-01

Examination of the fundamental relationship between chain confirmational changes and the macroscopic material responses during deformation. The program is based on the coupling of rheological and rheo-optical measurements during well characterized deformations. An in-situ infrared dichroism technique is used to study dynamically the molecular orientation during chain deformation and relaxation. Novel specimens that are partially deuterated allow the characterization of the deformation and relaxation behavior of essentially any segment of a polymer chain.

468. ASPECTS OF PHOTOIONIZATION OF IMPURITIES AND ELECTRON TRANSFER IN IONIC CRYSTALS

D. S. McClure
Dept. of Chemistry
Phone: (609) 452-4980

$86,600 03-1

Research of the relationship between the energy levels of impurity ions and the energy levels in the host crystal. Photoionization thresholds of impurity ions in crystals, such as Sm^{+2} in SrF_2, BaF_2, and CaF_2. Two photon spectroscopy in the strongly coupled ion-lattice system, $MgO:Ni^{+2}$. Studies of trapped excitons and phototransfer of electrons from one impurity ion to another.

PURDUE UNIVERSITY
West Lafayette, IN 47907

469. NOVEL POLYMERIC Li^+ AND DIVALENT CATION ION CONDUCTING MATERIALS: Li-SALT-IONENIC POLYMER SOLUTIONS, Li^+ CONTAINING PLASTIC CRYSTAL PHASES AND MI_2-$M(PO_3)_2$/$M(PS_3)_2$ GLASSES

C. A. Angell
Dept. of Chemistry
Phone: (317) 494-5256
E. I. Cooper
Dept. of Chemistry
Phone: (317) 494-5256

$78,762 01-1

Examination of the possibility of obtaining glasses with a relatively high conductivity in which the charge carrier is a divalent cation. Target systems include MI_2-$M(PO_3)_2$/$M(PS_3)_2$, where M^{2+} is Pb^{2+}, Cd^{2+}, or Sn^{2+}. Characterizations include measurements of electrical conductivity, nuclear magnetic resonance, internal friction, visco-elastic properties, and glass transition temperatures. Correlation of mechanical and electrical phenomena in mixed conduction systems such as mixed $Pb(PO_3)_3$-$PbBr_2$-$PbCl_2$ glasses and Na vanadate glasses.

470. MATERIALS RESEARCH UTILIZING NSLS

G. L. Liedl
School of Materials Engineering
Phone: (317) 494-4095

$545,000 01-1

This grant supports MATRIX, a group of 20 scientists from 9 institutions who have common interests in utilizing X-ray synchrotron radiation for unique materials research. This group has available to it 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 funds requested are to cover the operational expenses of this beam line at NSLS for all MATRIX members and to support part of the research on phase transformation studies and X-ray surface and interface studies.

PURDUE UNIVERSITY (continued)

471. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

A. A. Solomon
School of Nuclear Engineering
Phone: (317) 494-5753

$91,250 (23 months) 01-2

Study of elevated temperature tensile creep and stress rupture in well-characterized single phase ceramics in terms of rate controlling mechanisms and microstructural evolution. Experimental techniques consist of (1) tensile creep using constant true stress, (2) internal pressurization of pores with inert insoluble gas and microscopic measurement of pore or cavity growth under known hydrostatic pressure and surface tension driving forces. Results are correlated with quantitative microstructural studies of porosity evolution. Materials under investigation are CoO, UO_2, NiO, carbonyl Ni, and Si_3N_4.

472. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT DIFFUSION

M. A. Dayananda
School of Materials Engineering
Phone: (317) 494-4113

$77,000 01-3

The objectives are (1) to explore the role and development of zero-flux planes (ZFP) and flux reversals in both single phase and multiphase diffusion couples in multicomponent systems during isothermal diffusion, (2) to characterize the ZFP compositions in terms of diffusion paths and thermodynamic data, (3) to study the feasibility of regulating the inter-diffusion of elements with preferential development of ZFPs. Zero flux planes for individual components within the diffusion zone of either a single or multiphase multicomponent system have been identified. At ZFPs the interdiffusion flux of a given component goes to zero and exhibits reversal in its flow direction on either side of the plane.

PURDUE UNIVERSITY (continued)

473. STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA

H. Sato
School of Materials Engineering
Phone: (317) 494-4096
R. Kikuchi
School of Materials Engineering
Phone: (317) 494-4099

$96,026 01-3

Research on multicomponent diffusion under general chemical potential gradients. Application of the path probability method of irreversible statistical mechanics to analytically derive the Onsager relations for diffusion on an atomistic basis. The conditions treated are general enabling relations among measurable quantities under a variety of driving forces such as the Nernst-Einstein relation and the Haven ratio in multicomponent systems, to then be clearly understood. The general formalism of multicomponent diffusion and cross terms in the Onsager relations is examined, and the role of apparent vacancy flows and "wind" effects investigated. The method is applied to chemical diffusion problems in multicomponent systems and to understanding established empirical concepts such as "diffusion path" and "zero flux planes."

474. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION

J. G. Mullen
Dept. of Physics
Phone: (317) 494-3031

$57,000 02-2

A variety of condensed matter experiments using the 46.5 KeV Mossbauer transition in tungsten-183 produced at the Missouri University Research Reactor, which is a thousand times more intense than conventional Mossbauer sources. Quasi-elastic scattering in a liquid metal study of self-diffusion as a function of temperature; elastic-inelastic separation of the diffracted radiation in zinc to study large anomalous anharmonic contributions to the scattering; a determination of the charge density wave satellites in TaS_2 near the commensurate-incommensurate first order phase transition. An improved measurement of the asymmetry parameter of the 46.5 KeV transition. Experiments to separate the elastic and inelastic scattering at Bragg reflections for measurement of the quasi-elastic linewidths near critical points. Signal to noise for these experiments enhanced through the use of a specially developed microscopic conversion electron (MICE) detector: additional isotopes will be tried. In collaboration with W. B. Yelon and G. Shupp at the University of Missouri at Columbia.

PURDUE UNIVERSITY (continued)

475. A STUDY OF THE INTERACTION OF LIGHT WITH SUB-MICRON METALLIC SURFACES

R. G. Reifenberger
Dept. of Physics.
Phone: (317) 494-3032

$65,000 02-2

Interaction of visible and near-UV laser light with sub-micron metallic surfaces and with adatoms or adsorbates. Electrons from field emission tips are photo-emitted by a focused Argon-ion laser beam tuned to a particular wavelength and tunnel into vacuum through a surface potential barrier which is distorted by a strong applied electric field. The final state energy distribution analyzed for influence of electronic structure, of the quantum mechanical transmission through the barrier, and of the nature of photoexcitation at photon energies below the barrier top. Thermal effects of laser heating, laser assisted diffusion and laser induced desorption of adatoms.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, NY 12181

476. TESTS AND MODELING FOR SINTERING THEORY

R. H. Doremus
Dept. of Materials Engineering
Phone: (518) 266-6373
R. M. German
Dept. of Materials Engineering
Phone: (518) 266-6445

$82,000 01-1

Research on multicomponent diffusion under general chemical potential gradients. Application of the path probability method of irreversible statistical mechanics to analytically derive the Onsager relations for diffusion on an atomistic basis. The conditions treated are general enabling relations among measurable quantities under a variety of driving forces such as the Nernst-Einstein relation and the Haven ratio in multicomponent systems, to then be clearly understood. The general formalism of multicomponent diffusion and cross terms in the Onsager relations is examined, and the role of apparent vacancy flows and "wind" effects investigated. The method is applied to chemical diffusion problems in multicomponent systems and to understanding established empirical concepts such as "diffusion path" and "zero flux planes."

RENSSELAER POLYTECHNIC INSTITUTE (continued)

477. MECHANISM OF MECHANICAL FATIGUE IN FUSED SILICA

M. Tomozawa
Dept. of Materials Engineering
Phone: (518) 266-6451

$94,276 01-2

Mechanism of static fatigue and analysis of fatigue kinetics in fused silica. Measurement of diffusion coefficient and solubility of water into 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. Estimation of mechanical (static) fatigue kinetics by combining stress-accelerated diffusion and swelling data.

RICE UNIVERSITY
P. O. Box 1892
Houston, TX 77251

478. STUDY OF THE KINETICS AND THERMODYNAMICS OF HYDROGEN IN PD-BASED ALLOYS

R. B. McLellan
Dept. of Mechanical Engineering and Materials Science
Phone: (713) 527-4993

$75,605 01-3

Systematic measurements of the solubility, thermodynamic properties, and diffusivity of H atoms in the same Pd-based binary alloys. Low (270-350K) and high (500-1000K) temperature diffusion measurements respectively by a double-cell electrolyte system and the permeability time-lag method. Measurement of the temperature and pressure dependence of hydrogen solubility and the temperature and the substitutional solute concentration dependence of the elastic constants. Magnetic susceptibility and elastic constant measurements for Pd and Pd alloys. Statistical thermodynamic modeling. Theoretical models based upon Thiele moment expansions and cell cluster techniques for interstitial solid solutions containing secondary defects (e.g., vacancies).

RICE UNIVERSITY (continued)

479. APPLICATION OF SPIN-SENSITIVE ELECTRON SPECTROSCOPIES TO INVESTIGATIONS OF ELECTRONIC AND MAGNETIC PROPERTIES OF SOLID SURFACES AND EPITAXIAL SYSTEMS

G. K. Walters
Physics Dept.
Phone: (713) 527-4937
F. B. Dunning
Dept. of Physics
Phone: (713) 527-8101

$214,000 02-4

Spin polarized beams of electrons and metastable He(2^3S) atoms used in studies of surface magnetic behavior, dynamics of metastable deexcitation at surfaces, electronic properties of absorbed layers. Spin Polarized Low Energy Electron Diffraction (SPLEED) and Metastable Deexcitation Spectroscopy (MDS) investigations of magnetic properties of epitaxial systems at the monolayer level. Emphasis on monolayers of Cr on Au(110), and monolayers of V and Fe on Ag(001) for which theory predicts strongly enhanced two-dimensional ferromagnetic moments on metallic overlayers, interfaces and superlattices.

UNIVERSITY OF ROCHESTER
Rochester, NY 14627

480. FRACTURE TOUGHNESS OF MATERIALS

S. J. Burns
Dept. of Mechanical Engineering
Phone: (716) 275-4082

$76,960 01-2

Research on the relationships between deformation processes and phase transformations occurring at the tips of cracks and the fracture toughness of materials. Specific activities include observations of deformation structures at the tips of cracks in single crystals of LiF and Si, analysis of dislocation nucleation from tips of macroscopic cracks in a high-strength steel using crack-tip shields for the position of dislocations relative to the tips of cracks, thermomechanical measurements of phase transitions in ZrO_2 for phase transformation fracture toughening, and a thermodynamic analysis of thermal expansivity in materials.

UNIVERSITY OF ROCHESTER (continued)

481. MICROSTRUCTURAL BEHAVIOR OF NON-EQUILIBRIUM SYSTEMS

J. C. M. Li
Dept. of Mechanical Engineering
Phone: (716) 275-4038

$120,004 01-2

Coupled theoretical and experimental research on amorphous metals. Topics include: a) vacancies and interstitials introduced by energetic atoms, b) negative creep induced by a positive stress, c) crack extension and dislocation emission, and d) nucleation events in melting. Research also includes studies of rapidly crystallized structures.

ROCKWELL INTERNATIONAL SCIENCE CENTER
1049 Camino Dos Rios/Box 1085
Thousand Oaks, CA 91360

482. ADVANCED Si_3N_4 SYSTEM STUDIES

P. E. D. Morgan
Phone: (805) 373-4273

$224,924 01-5

Investigations of Si-S chemistry to provide starting points for the preparation of Si_3N_4 and SiC in various forms such as powder, whiskers, fibers, etc. Room temperature reactions of SiS_2 with hydrazine. TGA, XRD, TEM, NMR, IR, Fracture toughness.

RUTGERS UNIVERSITY
Busch Campus/P. O. Box 909
Piscataway, NJ 08854

483. LOCAL STRUCTURE OF METAL ATOMS IN SILICA AND SILICATES

S. H. Garofalini
Dept. of Ceramics
Phone: (201) 932-2216

$26,164 01-3

Local structure and bulk and surface diffusion of metal ions in vitreous silica and silicated glasses are investigated using a combination of X-ray extended fine structure (EXAFS) measurements and computer simulations using molecular dynamics methods. Studies include the effects of local structure, interatomic potential functions, atom size, ion clustering, and sample preparation on the mobility of metal species. Systems include alkali-zinc-silicates, sol-gel-prepared zinc silicates, and platinum on silica.

RUTGERS UNIVERSITY (continued)

484. HIGH PRESSURE AND SYNCHROTRON RADIATION STUDIES OF SOLID STATE ELECTRONIC INSTABILITIES

J. H. Pifer
Dept. of Physics
Phone: (201) 932-2524
M. C. Croft
Dept. of Physics
Phone: (201) 932-2522

$139,200 02-2

Studies of the configurational instabilities in 3d, 4f, and 5f compounds utilizing a novel high pressure diamond anvil electron paramagnetic resonance apparatus capable of operating at 100 kbar at liquid helium temperatures. Resistivity measurements and core level X-ray absorption studies using synchrotron radiation on both crystalline and amorphous mixed valence materials. Research on the $ThCr_2Si_2$ structure materials, with Th replaced by Ce and Eu to investigate the interplay of rare earth valence state with p-p bond formation. Investigation of heavy fermion regime with Cr replaced by $Mn_{1-x}Cr_x$. New amorphous rare earth compounds in thin films. Valence charge study of Ce in $Ce(Rh_xPd_{1-x})_3$.

SETON HALL UNIVERSITY
South Orange, NJ 07079

485. THE USE OF SURFACE CHARACTERIZED DISPERSED METAL CATALYSTS IN CATALYTIC REACTIONS

R. L. Augustine
Dept. of Chemistry
Phone: (201) 761-9033

$63,500 03-3

Extension of the single turnover reaction sequence developed for the surface characterization of Pt/CPG catalysts to characterize other catalysts and support combinations. The effects of the support on site specific reactivity will be determined. Support materials studied include alumina, silica, and titania. Metals studied include platinum, palladium, and rhenium.

SOUTHWEST RESEARCH INSTITUTE
6220 Culebra Road
San Antonio, TX 78284

486. CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION

R. A. Page
Dept. of Materials Science
Phone: (515) 684-5111 X3252
J. Lankford
Dept. of Materials Science
Phone: (515) 684-5111 X2317

$154,000 01-2

Characterization of pore evolution during sintering and cavitation during creep. Creep studies concerned with the effect of grain size, grain boundary phases, and choice of ceramic material with emphasis on compressive creep cavitation. Characterization of the effect of grain size and grain boundary chemistry upon the cavitation of pure Al_2O_3 subject to uniaxial tensile stress. Characterization of cavity development and breakaway conditions during the final stage sintering of Al_2O_3. Small angle neutron scattering to yield cavity nucleation and growth rates and average pore size, distribution, and morphology. TEM and precision density characterization. Modeling of cavitation and sintering behavior. Principal experimental materials: Al_2O_3, SiC.

SRI INTERNATIONAL
Menlo Park, CA 94025

487. MINOR ALLOYING ELEMENTS IN THE PITTING BEHAVIOR OF METALS AND ALLOYS

D. D. Macdonald
Chemistry Laboratory
Phone: (415) 859-3195

$128,908 01-3

Experimental and theoretical investigation of pitting in austenitic stainless steels (Fe-Cr-X-base composition). Extension of the solute/vacancy interaction model to consider breakdown of passive films and role of minor alloying elements thereon, modeling rate of generation of cation vacancies at the film/solution interface and the interaction between the solutes and vacancies for various solute types (effective valence and concentration). Experimental studies of breakdown characteristics of various alloys in aqueous chloride solutions and possibly other electrolytes. Application of results to alloy design.

STANFORD UNIVERSITY
STANFORD, CA 94305

488. INTERNAL-VARIABLE BASED MODELS FOR ELEVATED TEMPERATURE FATIGUE AND DEFORMATION

A. K. Miller
Dept. of Materials Science and Engineering
Phone: (415) 723-3732

$190,476 01-2

A program of research to develop a new unified computer model for elevated-temperature fatigue that will be based upon explicit representations of the controlling internal physical processes, and which will be completely quantitative and computer-based. Related research on the development of a physically-based model of the deformation and ductile failure behavior of metals and alloys, including development of improved constitutive equations for multiaxial plasticity, and a new model for sheet metal formability under nonproportional strain paths. This research advances earlier modeling work (the development of MATMOD and MATCON constitutive relations) on the plasticity of materials and serves as input to the elevated-temperature fatigue model.

489. MECHANISMS OF HIGH TEMPERATURE CRACK GROWTH IN METALS AND ALLOYS

W. D. Nix
Dept. of Materials Science and Engineering
Phone: (415) 497-4259

$98,619 (5 Months) 01-2

Study of the processes of creep crack extension in simple metals (Cu and Ni), examination of cavitation damage at crack tips using implanted intergranular cavities and intergranular segregation of Sb in Cu to permit grain boundary fracture in post-creep impact tests, study of the driving forces for crack growth and the temperature dependence of the growth process, examination of the effects of environments on creep crack growth in Ni alloys containing carbon, study of creep crack growth in 304 stainless steel containing different intergranular carbide distributions, theoretical studies of cavitation and crack growth.

STANFORD UNIVERSITY (continued)

490. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

R. H. Bube
Dept. of Materials Science and Engineering
Phone: (415) 497-2534

$210,000 01-3

Interactions occurring at the interface between CdTe with other materials, and the role of interfacial microstructure and microchemistry on the electrical properties of such CdTe containing heterojunctions. Effects of etching and heat treatment on surfaces, Schottky barriers, and heterojunctions formed on CdTe, and the preparation and behavior of polycrystalline films of CdTe. Grain boundary characterization and passivation. Measurements include J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; and diffusion lengths. Scanning transmission electron microscopy and high resolution and electron microdiffraction; XPS, Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition; magnetron sputtering; and chemical vapor deposition; and closed-space vapor transport techniques.

491. A STUDY OF MECHANICAL PROCESSING DAMAGE IN BRITTLE MATERIALS

B. T. Khuri-Yakub
Dept. of Electrical Engineering
Phone: (415) 497-0718

$102,701 01-5

The proposed research will investigate machining damage in brittle materials, initially hot-pressed Si_3N_4, and the associated residual surface stresses. Nondestructive evaluation (NDE) techniques will be developed and applied to the measurement of the depth of shallow cracks, simulating machining damage, and local stress fields. An attempt will be made to correlate the damage with microstructural features and to determine a quantitative relation between damage and remaining strength.

STANFORD UNIVERSITY (continued)

492. THE USE OF NON-DESTRUCTIVE EVALUATION TECHNIQUES IN THE STUDY OF SMALL FATIGUE CRACKS

D. V. Nelson
Dept. of Materials Science and Engineering
Phone: (415) 497-2123
J. C. Shyne
Dept. of Materials Science and Engineering
Phone: (415) 497-2123

$130,000 01-5

Study of the growth behavior of fatigue microcracks in 4140 and 300 M steels, as influenced by different microstructures. Monitoring of crack depth and variation in crack closure stress with crack growth using surface acoustic waves as a probe. Comparison of closure stress behavior with that determined by SEM measurements of crack mouth opening displacement vs. applied stress. Measurement by X-ray diffraction of changes in surface residual stresses during fatigue cycling. Correlation of crack growth rate with closure stress behavior, at different stress amplitudes and two mean stress levels. Investigation of the use of an acoustic microscope technique to furnish quantitative information about residual stresses.

493. A QUEST FOR A NEW SUPERCONDUCTING STATE

J. P. Collman
Dept. of Chemistry
Phone: (415) 497-4648
W. A. Little
Dept. of Physics
Phone: (415) 497-4233

$100,000 03-1

Synthesis and characterization of organic conductors in which the conducting spine is encompassed by macrocyclic dyes. Experimental tests of excitonic superconductivity. Preparation of polymeric materials consisting of stacked or bridged-stacked metalloporphyrin or metallophthalocyanine complexes. Structural characterization using EXAFS and XANES at the Stanford Synchrotron Radiation Laboratory and X-ray powder and single crystal crystallography. Measurements of conductivity, photoconductivity, and magnetic susceptibility. Calculations using extended Huckel molecular and band theory.

STEVENS INSTITUTE OF TECHNOLOGY
Hoboken, NJ 07030

494. SPIN POLARIZED PHOTOELECTRON STUDIES OF MAGNETIC IN SOLIDS

G. M. Rothberg
Dept. of Materials and Metallurgical Engineering
Phone: (201) 420-5269

$ 96,000 02-2

Magnetic order and the spin dependence of electron scattering in solids by means of a new technique, Spin Polarized Extended X-ray Absorption Fine Structure, or SPEXAFS. The spin polarization of electrons from exchange-split photoemission peaks used to observe EXAFS and obtain information about the distance and temperature dependences of spin-spin correlations in magnetic solids and on surfaces. Features of the photoelectron spectrum used such as ordinary EXAFS and the plasmon-loss peaks to obtain additional information. Photoemission EXAFS has a unique chemical sensitivity that make possible in Al-O systems the study of the atomic structure around an element in different chemical environments.

SYRACUSE UNIVERSITY
Syracuse, NY 13210

495. THE CATALYTIC REACTIVITY TO THIN FILM CRYSTAL SURFACES

R. W. Vook
Dept. of Physics
Phone: (315) 423-2564
J. A. Schwarz
Dept. of Chemical Engineering and Materials Science
Phone: (315) 423-4575

$171,607 01-1

Characterization of topography and defect structure on thin film surfaces (Pd, Pt) and of factors that determine their chemical reactivities, measurement of adsorption and desorption (thermal and electron beam induced) kinetics of O_2, CO, and hydrocarbons on these films, work function determination upon gaseous adsorption as a function of surface topography and defect structure, comparison of reactivities of vapor deposited thin film surfaces with similar surfaces that were sputter etched and annealed, chemical reaction investigations at elevated pressures using thin film samples as prototype catalysts that include the effects of catalytic promoters and poisons, techniques used - LEED, AES, EELS, TPD, TEM/TED, RHEED, work function.

UNIVERSITY OF TENNESSEE
Knoxville, TN 37996-1600

496. STATISTICAL MECHANICS OF POLYMER SYSTEMS

J. Kovac
Dept. of Chemistry
Phone: (615) 974-3444

$86,932 03-1

Theoretical investigation into the equilibrium and dynamic behavior of amorphous polymers over a broad range of concentration, molecular weight, and temperature. The investigations involve non-equilibrium thermodynamics, equilibrium and non-equilibrium statistical mechanics, and computer simulation. Specific problems include more realistic models for single chain dynamics, conformation and dynamics of chains in semi-dilute and bulk systems and equilibrium and dynamic aspects of the glass transition.

UNIVERSITY OF UTAH
Salt Lake City, UT 84112

497. EXPERIMENTAL STUDIES OF THE ELECTRONIC STRUCTURE OF I-II AND I-III INTERMETALLIC COMPOUNDS

I. M. Curelaru
Dept. of Materials Science and Engineering
Phone: (801) 581-4850, 3161

$86,580 01-1

Systematic investigation of the electronic structure of the occupied and empty states for I-II and I-III intermetallic Zintl compounds, with concern for the significance of nonstoichiometry, defect lattice, and degree of localization of conduction orbitals in determining physical behavior. Spectroscopic techniques consist of X-ray photoelectron spectroscopy (XPS), electron energy loss spectroscopy (EELS), core ionization loss spectroscopy (CILS), appearance potential spectroscopy (APS), and extended appearance potential fine structure (EAPFS). Comparison of XPS, EELS, CILS, and data with existing LCAO, cluster model, and self-consistent linear muffin tin LMT band-structure calculations.

UNIVERSITY OF UTAH (continued)

498. FABRICATION, PHASE TRANSFORMATION STUDIES AND, CHARACTERIZATION OF SIC-ALN-AL_2OC CERAMICS

A. V. Virkar
Dept. of Materials Science and Engineering
Phone: (801) 581-5396
R. Gohil
Dept. of Materials Science and Engineering
Phone: (801) 581-3781

$109,642 01-1

Preparation of SiC-AlN-Al_2OC powders by a carbothermal reaction of a mixture of SiO_2 and Al_2O_3 in N_2 or Ar. Fabrication of SiC-AlN-Al_2OC ceramics by hot pressing, and subjecting such dense, hot pressed ceramics to various annealing treatments. X-ray diffraction and STEM analysis to investigate phase equilibria, precipitate morphology, spinodal decompositions and grain boundaries especially with special regard to the nucleation and growth of possible grain boundary phases. Evaluation of room temperature bend strength and fracture toughness and elevated temperature creep. Emphasis on understanding the inter-relationship of fabrication, microstructure, and mechanical behavior.

499. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V QUATERNARY ALLOYS

G. B. Stringfellow
Dept. of Materials Science and Engineering
Phone: (801) 581-8387

$95,903 01-3

Development of an understanding of miscibility gaps in alloys including organometallic vapor phase epitaxial growth of metastable alloys. Effect of short range (100A to 1000A) clustering compositional inhomogeneity in $GaAs_{0.6}Sb_{0.5}$ alloys on hole and electron mobility and photoluminescence half-widths. Raman spectroscopy and STEM analysis of spinodal compositions and clustering.

VIRGINIA COMMONWEALTH UNIVERSITY
Richmond, VA 23284

500. INTERNATIONAL SYMPOSIUM ON THE PHYSICS AND CHEMISTRY OF SMALL CLUSTERS

P. Jena
Department of Physics
Phone: (804) 257-1313

$5,000 01-1

International symposium to be held on physics and chemistry of small clusters. Fundamental aspects of the structural, thermodynamic and electronic properties of small clusters will be examined. Discussions of practical applications will be included.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

501. STUDY OF THE EMBEDDED ATOM METHOD OF ATOMISTIC CALCULATIONS FOR METALS AND ALLOYS

R. A. Johnson
Department of Materials Science
Phone: (804) 924-6356

$73,200 01-1

Theoretical studies to (1) obtain a better physical insight into the relationship between the input data and the EAM model parameters, (2) study the effects which variation of the EAM model parameters have on predicted material properties, and (3) use these results to assess the range of applicability of the EAM model and to improve its reliability within this range.

502. MICROSTRUCTURAL EFFECTS ON THE FATIGUE BEHAVIOR OF FE-C-X ALLOYS

G. L. Shiflet
Dept. of Materials Science
Phone: (804) 924-6340
E. A. Starke Jr.
Dept. of Materials Science
Phone: (804) 924-6340

$81,717 01-2

This research project addresses the cyclic fatigue behavior of low alloy multiphase steels. The program will aim to establish the effect of microstructure on crack initiation and propagation in tensile and fatigue tests of steels with well-controlled and characterized microstructures. Parallel modeling of the phase stability and crack propagation is planned.

UNIVERSITY OF VIRGINIA (continued)

503. SURFACE STRUCTURE AND ANALYSIS WITH SCANNING TUNNELING MICROSCOPY AND ELECTRON TUNNELING SPECTROSCOPY

R. V. Coleman
Dept. of Physics
Phone: (804) 924-3781

$135,000 02-2

A scanning tunneling microscope (STM), operating at liquid nitrogen temperature, used to image atoms at surfaces of layer structure crystals and to detect the electronic rearrangement due to charge-density waves (CDW's). Further instrument development, and study of a wider range of CDW transitions. More detailed information on the CDW structure and how it modifies the STM image. Development of a similar instrument operating at liquid helium temperatures for the study of both CDW and superconducting transitions. Surface structure, defects and the early stages of oxidation using both instruments. Development of techniques for imaging surface absorbed molecules and eventual vibrational spectroscopy of such molecules. Continuing experiments on standard tunnel junctions using the STM to study the early stages of oxide and doped oxide barrier formation. STM studies to elucidate the localized atomic and localized electronic structure at surfaces and interfaces.

504. MAGNETIC IMPURITIES IN SUPERCONDUCTORS

J. Ruvalds
Dept. of Physics
Phone: (804) 924-6796

$115,400 02-3

Theoretical investigation of the influence of magnetic impurities on the critical magnetic field H_{c2} and other physical properties. Special attention given to the Chevrel phase superconductors and to the newly discovered material phases displaying field induced superconductivity. Emphasis on mechanisms to enhance high field behavior of superconductors. The response of charge density waves to electric and magnetic fields. Study of charge density waves in certain heavy Fermion systems.

WASHINGTON UNIVERSITY
St. Louis, MO 63130

505. NON-EMPIRICAL INTERATOMIC POTENTIALS FOR TRANSITION METALS

A. E. Carlsson
Dept. of Physics
Phone: (314) 889-5739

$42,000 (16 months) 02-2

Development of existing scheme for calculating interatomic potentials in simplified tight-binding models into a method applicable to transition metals and transition metal alloys with defects. Consideration of tight-binding models, the tight-binding parameters from a first principles band theory, and effects beyond the extant tight-binding model. Interatomic potentials tested both by experimental data and band theoretic calculations for surfaces and vacancies and subsequently used to calculate the properties of dislocations and grain boundaries.

UNIVERSITY OF WASHINGTON
Seattle, WA 98195

506. X-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls
Dept. of Physics
Phone: (206) 543-5900

$107,000 (15 months) 02-2

Investigation of the structure and behavior of materials at high pressure by measuring the Extended X-ray Absorption Fine Structure (EXAFS) utilizing synchrotron radiation. Focus on the behavior of materials exhibiting the mixed valent insulator-to-metal transformation, clearly apparent in their X-ray absorption spectra. Examination of the X-ray Absorption Near Edge Structure (XANES) in such materials, as well as others with pressure-sensitive phase transformations. Experiments at the Stanford Synchrotron Radiation Laboratory.

UNIVERSITY OF WASHINGTON (continued)

507. FUNDAMENTAL STUDIES OF ELASTOMERS

B. E. Eichinger
Dept. of Chemistry
Phone: (206) 543-1653

$103,500 03-1

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

508. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

B. R. Cooper
Dept. of Physics
Phone: (304) 293-3423

$61,000 03-1

Investigation of the crystallographic allotropes of elemental plutonium with detailed calculations of the electronic structure, including correlation effects and contributions to the lattice energy. Theoretical model based on hybridization of the 5f electrons with the band electrons. Studies of plutonium monpnictides and monochalcogenides, the plutonium alpha distorted fcc phase, magnetic ordering, electrical resistivity, and self-consistent surface electronic structure.

UNIVERSITY OF WISCONSIN/MADISON
Madison, WI 53706

509. STUDIES OF ALTERNATIVE-CRYSTALLIZATION-PHASE NUCLEATION

T. F. Kelly
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-1073

$95,950 (15 months) 01-1

Liquid-to-crystal nucleation theory to predict which of several crystalline phases will solidify from small droplets of metal alloys. An experimental program to produce and characterize these alternative crystallization phases. Droplet processing by electrohydrodynamic atomization, centrifugal atomization, and levitation melting. Thermal analysis and analytical electron microscopy of as solidified droplets. Comparison of experimental findings with predictions of liquid-to-crystal nucleation theory.

510. THE STABILITY OF AMORPHOUS METALS ON SEMICONDUCTOR SUBSTRATES

J. D. Wiley
Dept. of Electrical and Computer Engineering
Phone: (608) 263-1643
J. H. Perepezko
Dept. of Metallurgy and Mineral Engineering
Phone: (608) 263-1678

$87,340 01-1

Experimental investigation of the structure, stability, and atomic transport behavior of high-T amorphous-metal films on semiconductor substrates. RF sputtering deposition of thin amorphous films of Ni-Nb, Mo-Si, and W-Si alloys on semiconductor substrates of Si, GaAs, and GaP. Characterization of crystallization kinetics, crystallization mechanism, and film/substrate interdiffusion at temperatures near the glass-transition temperature by structural, calorimetric, and electrical measurements. Examination of structural relaxation by electrical resistivity measurements during post-deposition annealing. Measurement of diffusion and interdiffusion by a combination of Rutherford back scattering and Auger electron spectroscopy techniques. Assessment of reactions involving crystallization and possible phase separation, involving TEM analysis of in situ annealing, and supplementary SEM and X-ray diffraction measurements.

UNIVERSITY OF WISCONSIN/MADISON (continued)

511. THERMODYNAMICS AND KINETICS OF PHASE FORMATION OF THIN-FILM METAL ON GALLIUM ARSENIDE

Y. A. Chang
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-1821
M. G. Lagally
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-1821

$122,680 01-3

Investigate the thermodynamics and kinetics of phase formation for metal films deposited on GaAs. Investigation consists of (1) bulk phase equilibrium and thermodynamic determinations of selected Ga-As-M ternaries and the associated thermodynamic modeling and phase diagram calculations; (2) bulk diffusion-couple measurements of GaAs-M; and (3) lateral thin-film diffusion couple measurements of GaAs-M and thin-film studies of M on GaAs and of GaAs on M. Systems under investigation are Ga-As-Os, Ga-As-Pd, and Ga-As-W. Phase equilibrium determinations using X-ray diffraction, metallography, microprobe, differential thermal analysis (DTA) and differential scanning calorimetry (DSC). Thermodynamic properties for Ga-M compound phases measured using a solid-state emf method. Diffusion paths in GaAs-M determined by means of microprobe analysis with bulk diffusion couples. The thin-film lateral diffusion couples characterized primarily by electron microscopy. Reactions and phase formation in thin films of metal on GaAs and of GaAs on metal characterized by electron microscopy and a variety of thin-film compositional, microstructural, and crystallographic analysis.

512. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

W. M. Yen
Dept. of Physics
Phone: (608) 263-7475

$119,002 02-2

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

UNIVERSITY OF WISCONSIN/MADISON (continued)

513. ANALYSIS OF MICROPHASE SEPARATION IN ION CONTAINING POLYMERS

S. L. Cooper
Dept. of Chemical Engineering
Phone: (508) 262-1092

$233,050 (24 Months) 03-1

Investigations of the microstructure of several ionomer systems using techniques which probe different aspects of the structure. Development of a unified model of the morphology which can rationalize the unique physical properties of these materials. Of special interest, the Nafion[R] ionomers because of their applications in electrochemical processes as selectively permeable membranes. The local arrangement of atoms in the ionic domains studied using Extended X-ray Absorption Fine Structure (EXAFS) analysis and XANES spectroscopy. Information about larger scale structure obtained from X-ray scattering and transmission electron microscopy experiments. To better understand the reason for differences between various ion containing polymers, the effects of several composition and preparation variables explored.

UNIVERSITY OF WISCONSIN/MILWAUKEE
Milwaukee, WI 53201

514. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

S. Y. Tong
Dept. of Physics and Surface Studies Laboratory
Phone: (414) 963-4474

$90,428 02-3

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

SECTION C

Small Business Innovation Research

PHASE I SBIR PROJECTS

The goal of the Phase I projects is to determine the technical feasibility of the ideas proposed.

CERAMATEC, INC.
163 West 1700 South
Salt Lake City, UT 84115

550. HIGH THERMAL CONDUCTIVITY DISPERSION-STRENGTHENED SILICON NITRIDE

D. W. Richerson
Phone: (801) 486-5071

$ 49,848 (6 months) SBIR

Phase I will concentrate on evaluating the effects of adding 20 through 50% SiC particles and whiskers to Si_3N_4 starting materials and the effects of using alpha versus beta SiC. Baseline evaluation will include density, flexure strength, fracture toughness (K_{IC}), hardness and microstructure. Selected specimens will be further evaluated by thermal conductivity measurements and by actual testing as cutting tool inserts. Directions for optimization will be identified for study in Phase II.

FLOW RESEARCH COMPANY
21414 68th Ave. S.
Kent, WA 98032

551. CLUSTER BEAM TECHNOLOGY FOR THIN FILMS

A. C. Day
Phone: (206) 872-7080

$ 49,826 (6 months) SBIR

A systematic investigation of the Ionized Cluster Beam (ICB) deposition technique. Research will address the following: (1) how clusters are formed; (2) what the actual makeup is of a cluster beam; (3) how clusters and other beam species interact to form thin films; and (4) what intrinsic advantages ICB holds over other techniques. The Phase I approach will combine modeling and experimental work with an emphasis on front-end issues of beam generation and characterization. A limited series of thin films will also be grown and studied.

552. DEVELOPMENT OF HIGH-TEMPERATURE AMORPHOUS ALLOYS

R. Wang
Phone: (206) 872-7080

$ 49,845 (6 months) SBIR

Development of high-temperature amorphous intermetallic alloys with crystallization temperatures, T_x, as high as $1000^{o}C$ ($1273^{o}K$) for extended application in oxidation, sulfidation, corrosion, wear, and catalytic reactions. Phase I will establish criteria for quantitative interpretation and prediction of the crystallization temperature of binary amorphous intermetallic compounds and will develop two amorphous alloys designed to reach high thermal stability.

553. PROCESSING SCIENCE: UNDERSTANDING AND CONTROL OF THE WHISKER MATRIX INTERFACE IN CERAMIC-CERAMIC COMPOSITES

B. Sonupariak
Phone: (206) 872-7080

$ 49,964 (6 months) SBIR

This work will evaluate the feasibility of using processing science to tailor the composition and interface bonding of whisker-reinforced ceramic composites. Microstructural control will be evaluated by varying gel structures (colloidal versus polymeric) and sintering (liquid state versus solid state) conditions. The mullite-mullite and mullite-alumina composites were selected for the study of matrix-fiber interfaces because they provide the optimum characteristics for development of a model system. Work is planned to investigate the effects of microstructure and interface reactions on the fracture toughness and strength.

JUPITER TECHNOLOGIES
187 Langmuir Laboratories
Cornell Industrial Research Park
Ithaca, NY 14850

554. MECHANICAL RELIABILITY OF SUPERPLASTICALLY FORGED SILICON NITRIDE

P. C. Panda
Phone: (607) 257-4514

$ 50,000 (6 months) SBIR

This project will investigate whether forging improves the reliability of silicon nitride components. Phase I research will carry out a full-length statistical study and measure the Weibull modulus for superplastically forged silicon nitride.

OPTEL SYSTEMS
Optel Bar Code Systems, Inc.
317 Main Street
East Rochester, NY 14445

555. SURFACE FIGURE MEASUREMENTS OF X-RAY OPTICS

T. C. Bristow
Phone: (716) 385-6760

$ 49,867 (6 months) SBIR

This project will study the measurement of surface figure of X-ray mirrors and optical components. The proposed measurement technique will not contact the surface of the mirror and will be capable of a measurement during the polishing cycle. The technique also can measure a low-reflectance or uncoated surface. The effects of noise, focusing errors, and vibration will be studied for a stationary optic located on a polishing machine.

PHYSICAL OPTICS CORPORATION
3306 Dow Ave.
Redondo Beach, CA 90278

556. UV HOLOGRAPHIC MIRRORS WITH HIGH DIFFRACTION EFFICIENCY

J. Hannson
Phone: (213) 371-3909

$ 49,336 (6 months) SBIR

A new holographic approach is proposed for production of UV optical elements, which is based on nonlinear holographic recording of second-harmonic Bragg structure. This fabrication technique of UV optics will have at least two orders of magnitude lower cost than the conventional vacuum deposition technology. The high reflectivity of the holographic rugate mirror is achieved by a very large number of layers (up to 1000) formed in a single holographic recording.

SYN CRYS, INC.
122 E. Division Road
Oak Ridge, TN 37830

557. A SEARCH FOR METAL OXIDE-METAL NITRIDE EUTECTIC SYSTEMS

G. W. Clark
Phone: (615) 482-3411

$ 30,953 (6 months) SBIR

The chemical stability and the tendency for eutectic solidification will be explored for specific periodic group III and IV metal oxide-metal nitride systems. Blended oxide-nitride powders will be pressed into pellets, heated on W, Mo, or Ta strip heaters to form melts and then solidified. Free energy of formation data will be used to estimate the regions of existence and the chemical stability of these systems. Oxygen and nitrogen partial pressures will be maintained over melts and during the solidification process to enhance the coexistence of the oxides and nitrides. The high-temperature stability and solidification morphology for the systems Al_2O_3-TiN, Y_2O_3-TiN, ZrO_2-TiN, Al_2O_3-ZrN, Y_2O_3-ZrN, and ZrO_2-ZrN will be studied.

UNIVERSIAL ENERGY SYSTEMS, INC.
4401 Dayton-Xenia Road
Dayton, OH 45432

558. SURFACE MODIFICATION BY ION BEAM FOR IMPROVED CORROSION RESISTANCE

R. Bhattacharya
Phone: (513) 426-6900

$ 49,981 (6 months) SBIR

Development of a strongly corrosion-resistant amorphous layer on the surface of 304 stainless steel by the use of high-energy MeV ion beam processing. The best combination of ion parameters such as mass, energy, dose, and specific elemental addition for obtaining an amorphous layer will be determined. The aqueous corrosion behavior of the coated stainless steel will be investigated by standard electrochemical tests. The microstructural characterization and the corrosion kinetics will be studied by more advanced surface and electrochemical techniques.

PHASE II SBIR PROJECTS

The Phase II projects are a continuation of the successful Phase I projects. The goal of the Phase II projects is to determine commercial feasibility.

ADELPHI TECHNOLOGY
13800 Skyline Blvd.
Woodside, CA 94062

559. THE CONSTRUCTION OF A SOFT X-RAY SOURCE USING TRANSITION RADIATION FOR LITHOGRAPHY

M. A. Piestrup
President
Phone: (415) 851-0633

$478,564 (24 months) SBIR

Development of transition radiators with high average photon flux for X-ray sources. Investigation of the use of these sources for X-ray lithography in the production of integrated circuits. Measurement of total photon flux from several foil stacks using a newly developed high-average-current, 50 Mev accelerator. The radiators will be tested at full beam current for maximum flux and target lifetime.

ANALYSIS CONSULTANTS
21831 Zuni Drive
El Toro, CA 92630

560. THE DESIGN AND FABRICATION OF FLAT PANELS WITH HIGH ACOUSTIC TRANSMISSIVITY

B. G. Martin
President
Phone: (714) 380-1204

$490,000 (24 months) SBIR

Feasiblity of constructing media with high acoustic transmissivity for all frequencies. Program objectives are to determine theoretically the acoustic velocity profile which gives maximum transmissivity, to design flat test panels based on the theoretical results, and to fabricate test panels and measure the transmissivity vs. frequency from 0.5 MHz to 5MHz.

AMERICAN RESEARCH CORPORATION OF VIRGINIA
642 First St., P.O. Box 3406
Radford, VA 24143-3406

561. EDDY CURRENT NONDESTRUCTIVE EVALUATION OF LASER GLAZED METALLIC SURFACES

R. J. Churchill
President
Phone: (703) 639-9542

$245,132 SBIR

Eddy current nondestructinve evaluation techniques to characterize melt depth and to detect flaws in laser glazed metallic surfaces. Principal Phase I findings include a correlation between blaze depth and eddy current impedance plane phase angle, flaw detection using split core differential probe designs, and temperature effect characterization during on-line processing. Phase II objectives include an extension of eddy current/ material interaction theory, development of high temperature eddy current probe systems, design of rapid scanning laser glazing apparatus, establishment of signal processing techniques, finite element modeling, and the design, test, and optimization of a laser glazing prototype system. Findings will be incorporated in a closed loop laser processing system having multi-variable control based on eddy current NDE sensor technology.

CERAMATEC INC.
163 West 1700 South
Salt Lake City, UT 84115

509. PROCESSING AND CHARACTERIZATION OF SiCAlON CERAMICS

Raymond A. Cutler
Program Manager
Phone: (801) 486-5071

$232,486 SBIR

Liquid phase sintering of SiCAlON ceramics, with improved processing and compositional control, to yield ceramics with smaller critical flaws and higher strengths. Investigation of physical properties as a function of Al2OC content to demonstrate the ceramic engineering possible with SiCAl2OC. Novel sintering techniques to show economical densification of SiAlON ceramics. Elevated temperature strength and creep measurements to determine the temperature range where liquid phase sintered SiCAlON can be applied. Investigation of the stability of the solid solution in air, N_2, and Ar at temperatures up to 1700°C.

CERAMATEC INC.
163 West 1700 South
Salt Lake City, UT 84115

562. FABRICATION AND CHARACTERIZATION OF CERAMIC MATRIX-CERAMIC WHISKER COMPOSITES WITH RANDOM ORIENTATION OF THE WHISKERS

L. Viswanathan
Senior Research Scientist
Phone: (801) 486-5071

$498,816 (24 months) SBIR

Fabrication and charcterization of ceramic matrix-SiC whisker composites by pressureless sintering for advanced heat engines. Development of powder processing methods that yield randomly oriented whiskers. The materials to be studied are Al_2O_3 + SiC and Si-Al_2OC + SiC. The former is expected to retain toughness in excess of 8MPa $(m)^{1/2}$ in excess of 1000^oC and the latter to 1300^oC.

CERAMIC FINISHING COMPANY
P. O. Box 498
State College, PA 16804

564. FRACTURE MECHANICS INVESTIGATION OF GRINDING OF CERAMICS

Henry P. Kirchner
President
Phone: (814) 238-4270

$107,988 (24 months) SBIR

Application of contact fracture mechanics to investigate mechanisms of material removal and damage penetration during abrasive machining of ceramics. Phase I research investigated the mechanisms of material removal including crushing by mixed mode fracture ahead of the diamond point and chipping at lateral cracks propagating in response to residual stresses induced by elastic relaxation against the irreversibly deformed zone on unloading. The objective: determine the relative importance of crushing ahead of the diamond point and chipping alongside the track as a result of lateral cracking, for various material properties and grinding conditions, investigate the role of crushing in reducing the residual stresses that are responsible for lateral cracking, develop mathematical models by adapting available models for static indentations. The experimental results will be compared with results predicted by these models.

CERES CORPORATION INC.
202 Boston Road
North Billerica, MA 01862

565. HORIZONTAL GROWTH OF SILICON SHEET CRYSTALS VIA EDGE-SUPPORTED PULLING (ESP) FROM MELT CONTAINED IN A COLD CRUCIBLE

Joseph F. Wenckus
President
Phone: (617) 899-5522

$142,509 SBIR

Explore the feasibility of growing silicon sheet crystals horizontally using the edge-supported pulling (ESP) process from silicon melts contained in an RF heated crucible. The vertical ESP process provides exceptionally stable sheet growth conditions, but sheet growth rates achieved to date are severely restricted by the rate of heat dissipation from the narrow sheet/melt interface. This program endeavors to integrate the unique operational features of the cold crucible with the equally unique attributes of the ESP process to demonstrate the feasibility of the horizontal edge-supported pulling method for the production of silicon crystals.

ELECTROCHEMICAL TECHNOLOGY CORPORATION
3935 Leary Way, N.W.
Seattle, WA 98107

566. MATHEMATICAL MODELING OF ELECTROCHEMISTRY OF STRESS CORROSION CRACKING

T. R. Beck
Phone: (206) 632-5965

$164,149 (18 months) SBIR

Mathematical modeling of the electrochemical transport and kinetic processes that occur in tunnel corrosion of aluminum, correlative experiments on salt film properties using the shielded electrode technique, relation of the above to stress corrosion cracking.

KJS ASSOCIATES
1616 Hillrose Place
Fairborn, OH 45342

567. DEVELOPMENT OF ND-FE-B METAL-MATRIX MAGNETS

Reinhold M. W. Strnat
Research Engineer
Phone: (513) 299-0313, 2717

$171,149 SBIR

Heat-bonded composites of hard magnetic alloy powders in a ductile metal matrix fabricated and characterized for potential high energy permanent magnet applications. Refinement of techniques of comminuting, aligning, pressing, and bonding to produce good physical compacts that also have optimized magnetic properties. To prevent corrosion, grinding under protective gas and liquid will be tried with emphasis on minimizing the production of very fine particles. Methods to coat powders with elements like Zn, Sn, and Cu will be investigated. Modified magnetic materials such as Co- and Dy- containing Nd-Fe-B will be studied. Measurement of short-term reversible and long-term irreversible flux losses, long-term elevated temperature stability of magnetic flux, coercivity, and hysteresis loop shape. SEM and optical microscopy to characterize the bond between matrix and metal and magnetic constiturent after aging.

MATERIALS & ELECTROCHEMICAL RESEARCH CORP.
4660 N. Via Madre
Tucson, AZ 85749

568. THE DIRECT PRODUCTION OF INTERMETALLIC COMPOUND POWDER

J. C. Withers
Technical Manager
Phone: (602) 749-3257

$500,000 (24 months) SBIR

Examination of the feasibility of producing nickel and titanium aluminide intermetallic alloy powder by the direct reduction of metal chloride precursors. Definition of optimal operating conditions for producing Ni_3Al microalloyed with boron with and without hafnium and with uniform inter and intraparticle composition in a particle size useful in current powder-metallurgy processing. A continuous quartz reactor will be designed and operated for the purpose of establishing technical feasibility. The technical issues are to determine thermodynamically the most favorable operating conditions for phase control and material balance, to determine experimentally the optimum operating parameters for enhancing the nucleation of alloyed particles, to establish the need for microscopic mixing of product, and to develop an empirical model to describe nucleation kinetics.

SUPERCON INC.
9 Eric Drive
Natick, MA 01760

569. INVESTIGATION TO DETERMINE THE COMMERCIAL FEASIBILITY OF IN SITU CU-NB COMPOSITES FOR HIGH STRENGTH, HIGH CONDUCTIVITY APPLICATION

J. Wong
Phone: (617) 655-0500

$116,667 (24 months) SBIR

Development of a procedure for determining the commercial feasibility of fabricating 'in situ' Cu-Nb multifilamentary composites for high stress, high conductivity applications. Maintenance of a low volume fraction of Nb to retain desirable electrical and thermal properties of Cu. Evaluation of composite formability, tensile and fatigue strengths, and electrical conductivity.

SECTION D

Major User Facilities
(Large Capital Investment)

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, New York 11973

The National Synchrotron Light Source (NSLS) facility consists of a 750 MeV storage ring for VUV and IR research and a 2.5 GeV storage ring for X-ray research. Attractive features of synchrotron radiation include high brightness and intensity, broad and continuous spectral range, high polarization and pulsed time structure (subnanosecond pulses). Since each of the 28 X-ray and 16 VUV beam ports can be split into from 2 to 4 beam lines, as many as 100 experiments could run simultaneously at the NSLS. A 6 pole superconducting wiggler magnet and a 38 period permanent magnet undulator have been constructed, and several wiggler and undulator magnets are being designed which will significantly increase the photon intensity and brightness.

At NSLS a wide range of techniques are being used by solid state physicists, metallurgists, biologists, chemists, and engineers for basic and applied studies. Among the techniques are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

USER MODE

The policy for use of the NSLS is designed to enable the scientific community to cooperate in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines have been designed and instrumented by "Participating Research Teams" (PRTs). The PRTs are given priority for up to 75% of their beam line(s) operational time for a three-year term. Research groups are now forming insertion device teams (IDTs) to design and instrument beam lines and insertion devices.

General Users can perform experiments on an NSLS facility beam line or on a PRT beam line which, after an initial commissioning period, are available for use by non-PRT members for at least 25% of its total operational time. In the latter case, PRTs will provide liaison and utilization support to General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee is charged for the amount of beam time used. The DOE has granted the NSLS a Class Waiver, under the terms of which Proprietary Users of the NSLS will have the option to retain title to inventions that result from research performed at the NSLS.

Limited funding is 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 NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research and will be used to support only the most deserving cases.

PERSONS TO CONTACT FOR INFORMATION

Susan White-DePace (516) 282-7114
NSLS Department, Building 725B (FTS) 666-7114
Brookhaven National Laboratory

NATIONAL SYNCHROTRON LIGHT SOURCE

TECHNICAL DATA

Facilities	Key Features	Operating Characteristics
VUV electron storage ring	high brightness, continuous wavelength range (> 5Å) 16 beam ports.	0.75 GeV electron energy
X-ray electron storage ring	high brightness, continuous wavelength range (> .5Å) 28 beam ports	2.5 GeV electron energy

Instruments

Monochromators:	
plane grating	12Å < λ < 1500Å; high resolution
zone plate	8Å < λ < 100Å; moderate resolution
toroidal grating	10Å < λ < 2500Å; high intensity, moderate and high resolution
extended range grasshopper	10Å < λ < 2000Å; high resolution
Wadsworth	300Å < λ < 3000Å; high intensity, moderate resolution
Seya&Czerny Turner	1200Å < λ < 12000Å; high intensity, moderate resolution
two crystal	.04Å < λ < 2500Å; high resolution, fixed exit beam
two crystal/two grating	2.5Å < λ < 2500Å; high resolution, fixed exit beam
Six circle spectrometer/diffractometers	high positional and rotational accuracy
Experimental stations	photoemission, magnetic circular dichroism, fluorescence, gas phase spectroscopy, microscopy, lithography, holography, EXAFS, inelastic scattering, crystallography, radiometry, topography, small angle scattering
Permanent magnet undulator	30Å < λ < 5000Å; high intensity and brightness

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 particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths (> 4 Å). 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% 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 only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

D. Rorer (516) 282-4056
HFBR - Bldg. 750 FTS 666-4056
Brookhaven National Laboratory

HIGH FLUX BEAM REACTOR

TECHNICAL DATA

Instruments	Purpose and Description
Solid State Physics	
4 Triple-axis Spectrometers	Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 MeV, $< E_0 <$ 200 MeV Q range: $0.03 < Q < 10 Å^{-1}$
Biology	
Small Angle Neutron Scattering	Studies of large molecules. Located on cold source with 20 x 20 cm^2 position-sensitive area detector. Sample detector distance $L < 2$ meter. Incident wavelength $4 Å < \lambda_0 < 10 Å$
Diffractometer	Protein crystallography 20 x 20 cm^2 area detector $\lambda_0 = 1.57 Å$
Chemistry	
2 Diffractometers	Single-crystal elastic scattering 4-circle goniometer $1.69 Å < \lambda_0 < 0.65 Å$
1 Triple-axis Spectrometer	Inelastic scattering Diffuse scattering Powder diffractometry
Nuclear Physics	
3 Spectrometers	Neutron capture studies Energy range: $0.025 \text{ eV} < E_0 < 25$ KeV
TRISTAN II (Isotope Separator)	Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission
Irradiation Facilities	
7 Vertical Thimbles	Neutron activation; production of isotopes; thermal flux: 8.3×10^{14} neutrons/cm^2-sec; fast (>0.5 MeV) flux: 3×10^{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, fluxoid lattices in superconductors, liquid structures, and crystal structures. The HFIR is a 100-MW, light-water moderated reactor with an unsurpassed record of operating time (better than 90%). The central flux is 5×10^{15} neutrons/cm^2-sec, and the flux at the inner end of the beam tubes is slightly greater than 10^{15} neutrons/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.

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 six 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
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

(615) 574-5240
FTS 624-5240

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Technical Data

Beam No.	Instrument	Operating Characteristics
HB-1	Triple-axis polarized-beam	Beam size - 2.5 by 3 cm max Flux - 2.6 x 10^6 neut/cm^2 s at sample (polarized) Vertical magnetic fields to 5 T Horizontal fields to 2 T Variable E_0
HB-1A	Triple-axis, fixed E_0	E_0 = 14.7 MeV, 2.353 angstroms Beam size - 5 by 3.7 cm max Flux - 9 x 10^6 neut/cm^2 s at sample with 40 ft collimation
HB-2A	Liquid diffractometer with linear position sensitive detector	Beam size - 1 by 3.4 cm max Detector covers 130^0 scattering angle; Wavelength = 0.89 angstrom Flux - 6.8 x 10^5 neut/cm^2 s at sample with 20 min collimation
HB-2, HB-3	Triple-axis, variable E_0	Beam size - 5 by 3.7 cm max Flux - 10^7 neut/cm^2 s at sample with 40 min collimation
HB-3A	Double-crystal small-angle diffractometer	Beam size - 4 x 2 cm max Flux - 10^4 neut/cm^2 s Wavelength = 2.6 angstroms Resolution - 4 x 10^{-5} angstroms^{-1}
HB-4A	Four-circle diffractometer	Beam size - 5 x 5 mm Flux - 2 x 10^6 neut/cm^2 s with 9 min collimation Wavelength = 1.015 angstrom
	Wide-angle time-slicing diffractometer	Beam size - 2 x 3.7 cm max Flux - 2 x 10^6 neut/cm^2 s with 9 min collimation Wavelength=1.015 angstrom Curved linear position sensitive detector covering 130^0
HB-4	Correlation chopper	Beam size - 5 x 3.7 cm Flight path - 1.5 m 70 detectors covering 130^0 Variable E_0 Variable pulse width

INTENSE PULSED NEUTRON SOURCE

Argonne National Laboratory
Argonne, Illinois 60439

IPNS is an intermediate level pulsed spallation source dedicated to research on condensed matter. The peak thermal flux is about 3 x 10^{14} n/cm^2 sec. The source has some unique characteristics that promise to open 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

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 fundamental physics measurements as well as for technological applications, such as stress distribution in materials and characterization of zeolites, ceramics, and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS, Building 360, Argonne National Laboratory.

PERSONS TO CONTACT FOR INFORMATION

B. S. Brown, Acting Division Director	(312) 972-4999 FTS 972-4999
T. G. Worlton, Scientific Secretary	(312) 972-8755 FTS 972-8755

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

IPNS EXPERIMENTAL FACILITIES

NEUTRON SCATTERING

Facility (Instrument Scientist)	Assignment	Range Wave-vector	Range Energy	Resolution Wave-vector	Resolution Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-50 $Å^{-1}$	*	0.35%	*
General Purpose Powder Diffractometer (J. Faber, Jr., R. Hitterman)	F2	0.5-100 $Å^{-1}$	*	0.25%	*
Single Crystal Diffractometer (A. J. Schultz)	F6	2-20 $Å^{-1}$	*	2%	*
Low-Resolution Medium-Energy Chopper Spectrometer (C.-K. Loong)	F4	0.1-30 $Å^{-1}$	0-0.6 ev	0.02 k_0	0.05 E_0
High-Resolution Medium-Energy Chopper Spectrometer (D. L. Price)	H3	0.3-9 $Å^{-1}$	0.-0.4 eV	0.01 K_0	0.02 E_0
Small-Angle Scattering Diffractometer (J. E. Epperson, P. Thiyagarajan)	C1	0.006-0.3 $Å^{-1}$	*	0.004 $Å^{-1}$	*

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

NEUTRON BEAMS FOR SPECIAL EXPERIMENTS

Beam Tube	Current Use	Flight Path Length (m)
F3	eV Spectrometer	10
C2	Polarized Neutron Exp.	10
F1	n(P) Spectrometer	13.6
H1	Glass Diffractometer	10
H2	QENS Spectrometer	8

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 driven by the 800 MeV Los Alamos Meson Physics Facility (LAMPF) linear accelerator. Neutron scattering research is being carried out at LANSCE on six time-of-flight spectrometers. These are as follows: 1) a 32-m neutron powder diffractometer; 2) a single crystal diffractometer based on the Laue-TOF technique; 3) a filter difference spectrometer for chemical and optic mode spectroscopy; 4) a constant-*Q* spectrometer for studies of elementary excitations in single crystals; 5) a high intensity powder diffractometer, and 6) a low-Q diffractometer for small angle scattering studies which is located at a liquid hydrogen cold neutron source. A considerable effort is directed toward pulsed source instrument development including a chopper spectrometer, a neutron Anger camera and a back-scattering spectrometer for quasielastic scattering. The Proton Storage Ring (PSR) has reached 30% of its design intensity and will shortly enable LANSCE to deliver neutron pulses with the highest peak thermal flux for neutron scattering research in solid state physics, chemistry, biology and materials science.

USER MODE

During the initial start up of the PSR, LANSCE will operate in a collaborative mode. To propose an experiment, contact J. Eckert or the scientist responsible for the appropriate instrument. When the LANSCE facility is completed, it will be operated as a national user facility with formal proposals for experiments reviewed by a Program Advisory Committee (PAC) to allocate two-thirds of the available beam time. The PAC will evaluate proposals on the basis of scientific excellence and optimal use of LANSCE capabilities. One-third of the neutron scattering beam time is reserved for Laboratory discretionary research, research pertinent to DOE applied program goals, and instrument development. The LANSCE instrumentation is available without charge for nonproprietary research. The facility is open to all U.S. citizens and permanent resident aliens and to visits of less than seven working days for citizens of nonsensitive countries. DOE approval is required for any other foreign national visits.

PERSON TO CONTACT FOR INFORMATION

Juergen Eckert
MS H805, Group P-8
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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

LANSCE

TECHNICAL DATA 1986

Proton Source	LAMPF + PSR
Proton Source Current	1000 A
Proton Source Energy	800 MeV
LANSCE Proton Current	100 A
Proton Pulse Width	0.27 s
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 0.15%
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 94305

SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research in materials science, chemistry, biology, physics, engineering and medicine. 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, new ring designs). SSRL presently has 20 experimental stations. The radiation on nine stations is enhanced by insertion devices providing the world's most intense X-ray sources, and brightest soft X-ray source.

Commissioned in 1985 was the first experimental station on the 16 GeV storage ring, PEP. This line provides the world's most brilliant continuous X-ray beam, and will serve as a research tool and development center for future high-brilliance beam line concepts.

The primary research activities at SSRL are:

X-ray absorption, small and large angle scattering as well as topographic studies of atomic arrangements in complex materials systems, including surfaces, extremely dilute constituents, amorphous materials and biological materials.

Soft X-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter.

Non-invasive angiography. X-ray lithography and microscopy.

SSRL serves approximately 500 scientists from 110 institutions working on over 170 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. Access is gained through proposal submittal and peer review. In the course of a year approximately 70% 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 "General Information and Proposal Guidelines" includes information on proposal submittal and experimental station characteristics.

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell — (415) 854-3300 ext. 3191
SSRL, Bin 69 PO Box 4349 — (FTS) 461-9300 ext. 3191
STANFORD, CA 94305

CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

SSRL presently has 20 experimental stations 19 of which are located on SPEAR and one on PEP. Nine of these stations are based on insertion devices while the remainder use bending magnet radiation.

	Horizontal Angular Acceptance (Mrad)	Mirror CutOff (KeV)	Monochromator	Energy Range (eV)	Resolution $\Delta E/E$	Approximate Spot Size HgtxWdth (mm)	Dedicated Instrumenation
INSERTION DEVICE STATIONS							
WIGGLER LINES - X-RAY							
End Stations							
IV-2 (8 pole)							
Focused	4.6	10.2	Double Crystal	2800-21000	-5×10^{-4}	2.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	
VI-2 (54 pole)							
Focused	2.3	22	Double Crystal	2800-21000	-5×10^{-4}	2.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	
VII-2 (8 pole)							Six-circle Diffractometer
Focused	4.6	10.2	Double Crystal	2800-4500	-5×10^{-4}	1.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-21000	-10^{-4}	2.0 x 20.0	
Side Stations							
IV-1	1.0	-	Double Crystal	2800-45000	-5×10^{-4}	2.0 x 20.0	
IV-3	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	Two-circle Diffractometer
VII-1	1.0	-	Curved Crystal	6000-13000	-8×10^{-4}	0.6 x 3.0	Rotation Camera
VII-3	1.0	-	Double Crystal	2800-45000	-10^{-4}	2.0 x 20.0	
UNDULATOR LINES - VUV/SOFT X-RAY							
V-1	1.5	-	None	10-1200	≥7%	6.0 x 8.0	Variable Apertures
UNDULATOR LINES - X-RAY							
PEP 5B	Full	15.0	Double Crystal	12000-20000	-10^{-6}	0.6 x 6.0	
BENDING MAGNET LINES							
X-RAY							
I-4	2.2		Curved Crystal	6000-9500	- 60 eV	0.25 x 0.5	
I-5	1.0	-	Double Crystal	3800-29300	-10^{-4}	2.0 x 20.0	Area Detector/CAD-4
II-2 (focused)	4.8	8.9	Double Crystal	2800-8900	-5×10^{-4}	2.0 x 4.0	
II-3	1.0	-	Double Crystal	2800-30000	-5×10^{-4}	2.0 x 20.0	
II-4	1.0	-	None	3200-30000		4.0 x 15.0	
Lifetimes Port	1.8	-	None	1-6	Bandpass >10A	4.0 x .4	
VUV/SOFT X-RAY							
I-1	2.0		Grasshopper	32-1000	$\Delta\lambda$ = .1-.2A	2.0 x 1.0	
I-2	4.0		Seya-Namioka	4-40	$\Delta\lambda$ = .2-6A	1.0 x 3.0	
III-1	2.0		Grasshopper	15-1200	$\Delta\lambda$ = .05-2A	1.0 x 1.0	
III-3	8-10		Jumbo	800-4000	0.35-7 eV	2.0 x 4.0	
III-4	2.0		Multilayer	2-3000	White or $\Delta\lambda/\lambda$=.3%	2.0 x 11	Vacuum Diffractometer/ Exposure Station

Specialized Portable Beam Line Instrumentation Available: VG Chamber, Perkin Elmer Chamber, CAD-4, SAS Camera

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

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

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

M. Gillespie, Secretary NCSASR — (615) 574-5231
Oak Ridge National Laboratory — FTS 624-5231
Oak Ridge, Tennessee 37831

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: 10 m
Beam size at specimen: 0.5-3.0 cm diam
Sample-to-detector distance: 1.5-18.5 m
K range: $5 \times 10^{-3} \leq K \leq 0.6$ angstroms^{-1}
Detector: 64 by 64 cm^2
Flux at specimen: 10^4-10^6 neutrons/cm^2 s depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite
Incident wavelengths: 1.542 angstoms (CuK_{alpha}) or 0.707 angstoms (MoK_{alpha}) Source-to-sample distances: 0.5, 1.0, 1.5 . . ., 5.0 m
Beam size at specimen: 0.1 by 0.1 cm (fixed)
Sample-to-detector distances: 1, 1.5, 2.0 . . . ., 5 m
K range covered: $3 \times 10^{-3} \leq K \leq 0.3$ angstoms^{-1} (CuK_{alpha})
$6 \times 10^{-3} \leq K \leq 0.6$ angstoms^{-1} (MoK_{alpha})
Maximum flux at specimen: 10^6 photons per second on sample-irradiated area 0.1 by 0.1 cm^2
Detector: 20- by 20-cm^2 (electronic resolution 0.1 by 0.1 cm^2)
Special features: deformation device for dynamic scattering experiments (time slicing in periods as short as 100 microseconds for oscillatory experiments or 10 s 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 300 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 600 kV injector is underway as a replacement for the 300 kV 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), and a Philips EM 420 TEM/STEM equipped with XEDS and an electron energy loss spectrometer (EELS). A Philips EM430 with an XEDS will be added shortly. 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 AES. As such, it will have substantially increased analytical capabilities for materials research over present-day instruments.

USER MODE

The Center 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
H. Wiedersich (312) 972-5079
Electron Microscopy Center for Materials Research FTS 972-5079
Materials Science and Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

TECHNICAL DATA

Electron Microscopes	Key Features
High-Voltage Electron Microscope Kratos/AEI EM7 (1.2 MeV)	Resolution 3.5 Å lattice Continuous voltage selection (100-1200 kv) Current density 15 A/cm^2 High-vacuum specimen chamber Negative-ion trap Electron and ion dosimetry systems Video recording system Ion-beam interface Specimen stages 10 - 1300 K Straining and environmental stages
Transmission Electron Microscope Philips EM 420 (120 keV)	Resolution 2.0 Å lattice Equipped with EELS, XEDS Specimen stages 15 - 300 K
Transmission Electron Microscope JEOL 100 CX (100 keV)	Resolution 2.0 Å lattice Equipped with STEM, XEDS Specimen stages 300 - 900 K
Analytical Electron Microscope Being acquired (300 keV)	State-of-the-art resolution Ultra-high vacuum, Field Emission Gun Equipped with EELS, XEDS, etc.

Accelerators	
NEC Model 2 UDHS	Terminal voltage 2 MV Energy stability $\pm$250 eV Current density: H^+, 10 μA/cm^2 (typical) Ni^+, 3 μA/cm^2
Texas Nuclear 300-kV	Terminal voltage 300 kV Energy stability $\pm$300 eV Current density: He^+, 200 μA/cm^2 (typical) Ni^+, 2 μA/cm^2
NEC 600 kV Injector Being acquired	Terminal voltage 600 kV Energy stability $\pm$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

The microanalysis facilities for use in materials science have been made 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, field ion microscopy/atom probe, 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. An intermediate high voltage analytical electron microscope (300 kV) and an atom probe field ion microscope have been recently added to the SHaRE facilities.

USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, P. S. Sklad, R. J. Bayuzick, R. F. Davis, and R. E. Wiesehuegel. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and current ORNL research. One ORNL staff member must be identified who is familiar with required techniques and will share responsibility for the project.

The SHaRE program provides technical help and limited travel expenses for academic participants through the Oak Ridge Associated Universities (ORAU).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik — (615) 574-5066
Metals and Ceramics Division — FTS 624-5066
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

A. Wohlpart — (615) 576-3422
Oak Ridge Associated Universities — FTS 626-3422
P. O. Box 117
Oak Ridge, Tennessee 37831

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Facilities	Key Features	Operating Characteristics*
Hitachi HU-1000 High Voltage Electron Microscope	Heating stages; in situ deformation stages; videorecording system; environmental cell	0.3-1.0 MeV; in situ studies electron irradiation studies; ten 4-h shifts per week
Philips EM400T/ FEG Analytical Electron Microscope (AEM)	EDS, EELS, CBEB, STEM; minimum probe diameter ~1 nm	120 kV; ten 4-h shifts per week; structural and elemental microanalysis
JEM 120CX (AEM)	EDS, EELS, CBED, STEM; minimum probe diameter <10 nm	120 kV; ten 4-h shifts per week; structural and elemental microanalysis
JEM 120C TEM	Polepiece for TEM of ferromagnetic materials	120 kV; ten 4-h shifts per week; structural microanalysis
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 micrometer beam; hot-cold fracture stage; RGA; depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Dual Ion-Beam Accelerator Facilities	400 kV, 4 MV Van de Graaf accelerator; sputter profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis
Philips EM430T AEM	300 kV, STEM, EDS, EELS, CBED	Ten 4 h shifts/week; structural and elemental microanalysis
Atom Probe Field Ion Microscope	FOF atom probe, imaging atom probe, FIM, pulsed laser atom probe	Atomic resolution imaging; single atom analysis;

*Many instruments available off-hours (evenings, weekends) to qualified users.

CENTER FOR MICROANALYSIS OF MATERIALS

Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

The Center operates a wide range of advanced surface chemistry, X-ray and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, microcrystallography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded by MRL contracts of U 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 facility users has to be in the furtherance of DOE objectives.

The facility 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.

A brochure describing the Center and its services is available.

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	Features and Characteristics
Imaging Secondary Ion Microprobe Cameca IMS 3f	Dual ion sources (C_s^+, O_2^+). 1μm resolution.
Secondary Neutral Mass Spectrometer Leybold Heraeus INA 3	Quantitative analysis, Depth profiling.
Scanning Auger Microprobe Physical Electronics 595	Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector.
Scanning Auger Microprobe Physical Electronics 545	Resolution: SEM 3 μm.
XPS Physical Electronics 548	Double pass CMA. ESCA and Auger Specimen temp. to 1550K
Transmission Electron Microscope Philips EM430 (300kV)	EDS, EELS, STEM
Transmission Electron Microscope Philips EM420 (120kV)	EDS (windowless), EELS, STEM, Cathodoluminescence, Cold Stage (30K).
Transmission Electron Microscope Philips EM400T (120kV)	EDS. Heating, cooling stages.
Transmission Electron Microscope JEOL 4000EX (400 kV)	For environmental cell use.
Scanning Transmission E.M. Vacuum Generators HB5 (100kV)	0.5 nm probe, field emission gun, EDS, EELS.
Scanning Electron Microscope JEOL JSM 35C (35kV)	5 nm resolution, EDX, channeling and backscattering patterns.
Rutherford Backscattering (in-house construction) (3 MeV)	Two work stations, channeling
X-ray Equipment Elliott 14 kW high brilliance source Rigaku 12 kW source Several conventional sources Rigaku D/Max-11B Computer Controlled Powder Diffractometer	4-circle diffactometer. Small angle camera. EXAFS. Lang topography, Powder cameras, etc.

In addition to the main items listed above 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.

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.

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. Through in situ analysis by ion beam, surface, and bulk properties techniques, the fundamental materials interactions leading to these property changes are determined. Since both ion implantation doping and pulsed-laser annealing are nonequilibrium processing techniques, they can be used to produce new and often unique materials properties not possible with equilibrium fabrication techniques. This makes them ideal tools for fundamental materials research. They are equally useful for modifying 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 — (615) 576-6719
Solid State Division — FTS 626-6719
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

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, D, ^{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 most species to 7 MeV
10-200-KV high-current ion Implantation Accelerator	Essentially any species of ion; 1-3 mamps singly charged, ~100 microamps doubly and triply charged
0.1-10-KeV Ion Gun	Gaseous species; ~20 microamps
Lasers	
Pulsed Ruby Laser (0.6943 micrometer)	15-30 x 10^{-9} s pulse duration time; 10 joule/pulse output multimode; 2 joule/pulse output single mode (TEM_{00})
Pulsed Ruby Laser (0.6943 micrometer)	15-30 x 10^{-9} s pulse duration time; 8 joule/pulse output single mode (TEM_{00})
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; liquid helium cryostat; UHV goniometers (4-1300 K)
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 processing	Laser and ion beams integrated into same UHV chambers
Dual simultaneous ion-beam irradiations	Combined accelerator irradiations

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94550

Optical techniques, primarily Raman spectroscopy and nonlinear optical spectroscopy, are being developed and used to study high-temperature interactions of materials exposed to combustion 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. Combustion flow reactors and laboratory furnaces equipped with convenient optical accesses provide 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, are being developed for the detection of monolayer and submonolayer coverages of surfaces. Picosecond Nd:YAG and dye lasers (10 pps) and a high repetition rate (1kHz) Nd:YAG laser provide pulsed excitation at a variety of wavelengths. Analysis of samples in UHV-based systems provides careful control over the high temperature modification of surfaces.

USER MODE

The materials program at the Combustion Research Facility has emphasized research into deposition and corrosion mechanisms using the techniques and apparatus described above. Interactions include: (1) collaborative research projects with outside users, and (2) technology transfer of new diagostic approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the persons listed below. If further investigations appear reasonable, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government laboratories have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSONS TO CONTACT FOR INFORMATION

Marshall Lapp, High Temp. Interfaces Div. (8352) (415) 422-2435
FTS 532-2435

Gary B. Drummond, Ass't to the Director (8301) (415) 422-2697
FTS 532-2697

Sandia National Laboratories
Livermore, California 94550

TECHNICAL DATA

Instruments	Key Features	Comments
Raman Surface Analysis System	UHV Chamber; Raman system with Ar laser; triple spectrograph, diode array detector and 2-D imaging photon counting detector; Auger; sputtering capability.	Simultaneous Raman and sputtering. Raman system capable of detecting 2 nm thick oxides. Sample heating up to 1100 C.
Raman Microprobe	Hot stage; Raman system with Ar, Kr lasers; scanning triple spectrometer.	1-2 micron spatial resolution. Hot stage can handle corrosive gases.
Raman High-Temperature Corrosion System	Furnace; Raman system with Ar, Kr, Cu-vapor lasers Nd:YAG;triple spectrograph and diode array detector.	Pulsed lasers gated detection for blackbody background rejection. Furnace allows exposure to oxidizing, reducing, and sulfidizing environments.
Combustion Flow Reactors	Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and diode array detector.	Vapor and particulate injection into flames. Real-time measurements of deposit formation.
Electrochemical Surface Modification System	Electrochemical cell; Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and diode array detector.	Electrochemical cell with recirculating pump and nitrogen purge.
Nonlinear Optical Spectroscopy of Surfaces System	Picosecond Nd:YAG and dye lasers, 10 pps; UHV chamber equipped with LEED, Auger, sputtering, and quad. mass spectroscopy.	Monolayer and submonolayer detection of high temperature hydrogen and oxygen adsorption and nitrogen segregation on alloys.
Nonlinear Optical Spectroscopy of Electrochemical Systems	Nd:YAG laser, 1kHz rep rate; electrochemical cell.	Monolayer and submonolayer detection of lead,oxygen, and hydrogen adsorption at electrodes.

MATERIALS PREPARATION CENTER

Ames Laboratory
Iowa State University
Ames, Iowa 50011

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section and the Materials Referral System and Hotline (MRSH). 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.

USER MODE

Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Frederick A. Schmidt, Director, Materials Preparation Center.

Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquiries should be directed to Tom Wessels, MRSH Manager, (515) 294-8900 or FTS 865-8900.

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 (ARM), a high-resolution feeder microscope (JEOL 200 CX), and a 200-kV analytical microscope (JEOL 200 CX) equipped with a thin window, high-angle X-ray detector, and an energy loss spectrometer. Facilities for image simulation, analysis and interpretation are also available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. J. J. Hren, Chairman; J. M. Gibson, D. A. Howitt, F. Ponce, J. C. H. Spence, C. W. Allen, and L. E. Thomas; internal members are G. Thomas, T. L. Hayes, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be a sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer, and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore
National Center for Electron Microscopy
Mail Stop: 72-150
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

(FTS) 451-5006, or
(415) 486-5006

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characterization
KRATOS 1.5-MeV Electron Microscope	Resolution 3 A (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 A (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, $\pm 40^o$ 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 A 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 A (pt-pt) U.H. resolution goniometer stage only.	200 kV only, LaB_6 filament, 2.3-mm or 3-mm diameter specimens.
JEOL 200 CX dedicated Analytical Electron Microscope	Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, EELS spectrometer.	100 kV-200 kV LaB_6 filament, state-of-the-art resolution; 3-mm diameter specimens.

LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The Low-Temperature Neutron Irradiation Facility (LTNIF) is a user-oriented facility for the study of radiation effects in materials. It is available for qualified experiments at no cost to users. The LTNIF provides a combination of high radiation intensities and special environmental and testing conditions that have not been previously available in the U.S. A closed-cycle liquid-helium refrigerator and other cooling equipment allows samples to be held at temperatures between 3.2 and 800 K during irradiations and tests. In the initial configuration, the irradiation chamber fits into a vacant fuel element position in the reactor core to optimize fast neutron flux. Spectrum modifiers will be designed and constructed as needed to optimize gamma-ray or thermal-neutron flux. In many cases, experimental characterizations can be carried out in the irradiation cryostat. Alternatively, cold transfer to auxiliary equipment is available. The conditions available in the LTNIF are expected to prove useful in a wide variety of radiation effects studies, ranging from measurements of defect production and characterization in materials to the production of nonequilibrium phases of solids and the evaluation of structural materials for use in fusion reactors.

USER MODE

The LTNIF is operated as a user-oriented facility. In addition, a limited number of collaborative research projects will be undertaken by the staff. Time on the facility is assigned on the basis of proposals submitted in advance. Staff members are aided in the selection of user experiments by an advisory/program committee. Because of the special safety requirements of operating in a reactor, acceptance of proposals requires an evaluation by appropriate ORNL safety personnel in addition to the usual evaluation for scientific merit. Use of the reactor and cryostat is at no cost to users, but extensive use of shops and other support facilities must be paid by the user.

PERSONS TO CONTACT FOR INFORMATION

H. R. Kerchner — (615) 574-6270
Solid State Division — FTS 624-6270
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37831

R. R. Coltman, Jr. — (615) 574-6263
Solid State Division — FTS 624-6263
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37831

NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Technical Data

Refrigeration:	Minimum temperature, 3.2 K (low reactor power) Capacity at 5 K, 70 W (removes nuclear heat generated in cryostat and a 100 g experiment at full reactor power)
Radiation (preliminary):	Fast neutrons, (E > 0.1 MeV) 2×10^{17} n/m^2s Thermal neutrons, 1.5×10^{17} n/m^2s Gamma rays, 0.3 w/g (in Al)
Dimensions:	Irradiation chamber, 38 mm diam x 250 mm long Test chamber, 198 mm diam x 300 mm long

SECTION F

Summary of Funding Levels

SUMMARY OF FUNDING LEVELS

During the fiscal year ending September 30, 1986, the Materials Sciences total support level amounted to about $134.4 million in operating funds (budget outlays) and $12.0 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. In contrast, 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	28.1
(b) South................... (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	11.2	18.9
(c) Midwest................. (IA, IL, IN, MI, MN, MO, OH, WI)	21.8	28.9
(d) West.................... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	29.2	24.1
	100.0	100.0

2. By Discipline:

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Number 01-)	57.6	36.4
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	34.2	52.2

SUMMARY OF
FUNDING LEVELS

	Contract and Grant Research (% by $)	Total Program (% by $)
(c) Chemistry, Chemical Eng. (Budget Activity Numbers 03-)	8.2	11.4
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including laboratories where graduate students are involved in research to a large extent, i.e., LBL, Ames and IL)...	34.1
(b) DOE Laboratory Programs...........	64.1
(c) Industry and Other................	1.8
	100.0

4. By Laboratory and Contract and Grant Research:

	Total Program (%)
Ames Laboratory	5.3
Argonne National Laboratory	16.4
Brookhaven National Laboratory	20.6
Idaho National Engineering Laboratory	0.3
Illinois, University of (Materials Research Laboratory)	2.7
Lawrence Berkeley Laboratory	9.3
Lawrence Livermore National Laboratory	0.9
Los Alamos National Laboratory	3.2
Oak Ridge National Laboratory	16.6
Pacific Northwest Laboratory	1.1
Sandia National Laboratory	4.0
Solar Energy Research Institute	0.2
Stanford Synchrotron Radiation Laboratory	0.8
Contract and Grant Research	18.6
	100.0

SUMMARY OF
FUNDING LEVELS

5. By Selected Areas of Research:

	% of Prorated Projects[a] (Total=425)	% of Program Funding[a] ($134.4 million)	% of Individual Projects[c] (Total=425)
Materials			
Ceramics (Crystalline)	15.3	12.6	21.6
Ferrous Alloys	8.3	4.9	16.7
Intermetallics	2.8	3.8	9.8
Polymers	3.9	2.6	6.8
Semiconductors	6.4	6.0	16.7
Technique			
Electron Microscopy (Technique Development)	4.1	4.3	11.5
Neutron Scattering	5.9	19.1	16.2
Synchrotron Radiation	5.4	14.1	10.8
Theory	13.4	8.1	33.4
Phenomena			
Catalysis	2.2	2.2	6.6
Corrosion	3.6	2.3	9.9
Diffusion	4.2	3.4	16.9
Processing Science/Synthesis[b]	8.3	7.4	34.6
Strength	8.0	4.4	27.8
Superconductivity	2.6	3.1	7.8
Environment			
High Temperature (> $1200^{o}K$)	5.5	6.9	8.0
Radiation	6.4	9.4	10.6
Sulfur-Containing Gases	0.8	0.8	1.6

[a]The funding levels and projects percentage for various research categories were determined from the index listing in Section G and estimating the percentage from the project devoted to a particular subject. There is no overlap in the figures. For instance, funding for a project addressing creep of oxides would appear in the categories of ceramics, strength, and (possible) high temperature.

[b]Based on projects indexed in Section G under coatings, materials, preparation, powder metallurgy, solidification, surface treatments, thin films, and welding.

[c] Percentage of sum of individual projects involving the designated area of materials research.

SECTION G

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

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

MATERIALS, TECHNIQUES, PHENOMENA, AND ENVIRONMENT

The numbers in parenthesis at the end of each listing of Abstract numbers gives for each topic the percentage of prorated projects, the percentage of funding, and the percentage of individual projects respectively. The prorated projects and the funding levels are based on estimates of the fractions of a given project devoted to the topic. The operating funds for fiscal year 1986 were $134,455,000, and the total number of projects was 425.

MATERIALS

Actinides-Metals, Alloys and Compounds
006, 008, 014, 048, 049, 054, 076, 164, 200, 205, 241, 244, 255, 323
349, 366, 417, 424, 508
(1.46, 1.43, 4.47)

Aluminum and its Alloys
019, 078, 106, 107, 109, 113, 126, 142, 175, 190, 201, 218, 232, 291
310, 316, 318, 321, 344, 356, 363, 427, 488, 497, 566
(2.00, 1.34, 5.88)

Alkali and Alkaline Earth Metals and Alloys
081, 164, 166, 206, 241, 373, 420
(0.38, 0.40, 1.65)

Amorphous State: Liquids
058, 128, 131, 164, 245, 260, 306, 352, 428, 465
(0.96, 0.50, 2.35)

Amorphous State: Metallic Glasses
001, 043, 045, 075, 078, 106, 107, 123, 140, 191, 200, 201, 218, 223
232, 255, 277, 312, 321, 348, 365, 384, 406, 430, 449, 481, 510, 558
(2.16, 1.82, 6.59)

Amorphous State: Non-Metallic Glasses (other than Silicates)
041, 047, 054, 081, 118, 119, 120, 152, 200, 227, 235, 277, 304, 317
333, 341, 348, 368, 406, 410, 415, 418, 426, 436, 469, 484, 496, 512
552
(2.12, 1.67, 6.82)

Amorphous State: Non-Metallic Glasses (Silicates)
012, 054, 116, 260, 262, 275, 303, 406, 418, 425, 436, 450, 477, 483
512
(1.29, 1.44, 3.53)

Nitrides
012, 021, 022, 056, 120, 178, 204, 229, 264, 303, 342, 346, 376, 388
397, 411, 412, 440, 482, 491, 498, 550, 554, 557
(1.67, 1.05, 5.65)

Oxides: Binary
021, 041, 047, 055, 058, 079, 081, 117, 118, 121, 144, 149, 151, 153
167, 201, 204, 218, 220, 229, 231, 235, 242, 244, 245, 260, 292, 301
303, 317, 330, 333, 342, 343, 346, 353, 359, 374, 375, 376, 382, 383
384, 387, 388, 389, 396, 401, 407, 412, 427, 432, 433, 435, 445, 451
453, 464, 466, 470, 471, 476, 480, 483, 486, 490, 494
(5.44, 4.29,15.76)

Oxides: Non-Binary, Crystalline
021, 044, 049, 079, 116, 117, 127, 144, 147, 149, 151, 154, 218, 229
231, 235, 245, 260, 263, 292, 304, 333, 338, 342, 346, 353, 357, 376
377, 386, 388, 396, 407, 410, 432, 435, 445, 448, 455, 485, 553, 557
562, 563, 564
(3.22, 2.12,10.59)

Polymers
022, 084, 132, 177, 204, 224, 232, 236, 243, 255, 280, 307, 327, 345
351, 359, 362, 367, 409, 418, 422, 436, 438, 467, 469, 493, 496, 507
513
(3.91, 2.61, 6.82)

Platinum Metal Alloys (Platinum, Palladium, Rhodium, Irridium, Osmium, Ruthenium)
002, 015, 129, 142, 291, 335, 349, 355, 403, 478, 483, 485, 495, 511
(1.41, 0.70, 3.29)

Quantum Fluids and Solids
013, 047, 054, 128, 158, 161, 164, 166, 206, 223, 315, 322, 331, 352
369, 392, 403
(1.46, 1.19, 4.00)

Radioactive Waste Storage Materials (Hosts, Canister, Barriers)
116, 200, 263, 304, 386, 388, 410, 448, 457, 483
(0.71, 0.24, 2.35)

Rare Earth Metals and Compounds
001, 002, 003, 005, 006, 008, 010, 011, 014, 015, 018, 048, 054, 075
076, 141, 164, 166, 205, 223, 225, 235, 241, 323, 341, 372, 403, 408
416, 424, 468, 484, 504, 506
(2.35, 2.29, 8.00)

TECHNIQUES

<u>Elastic Constants</u>
049, 050, 072, 112, 126, 175, 201, 336, 353, 354, 377, 443, 452, 478
(0.73, 0.51, 3.29)

<u>Electrochemical Methods</u>
005, 024, 057, 058, 059, 060, 105, 131, 132, 160, 165, 168, 170, 242
260, 261, 280, 329, 337, 338, 340, 356, 379, 395, 398, 401, 436, 447
487, 511, 558, 566
(2.92, 2.25, 7.53)

<u>Electron Microscopy (technique development for all types)</u>
002, 003, 004, 041, 043, 044, 056, 070, 106, 107, 109, 110, 111, 113
115, 119, 122, 140, 141, 142, 143, 146, 148, 172, 174, 175, 190, 200
201, 202, 202, 217, 218, 219, 220, 227, 228, 234, 240, 256, 260, 301
358, 363, 375, 432, 439, 441, 480
(4.14, 4.23,11.53)

<u>Electron Spectroscopy for Chemical Analysis (ESCA)</u>
023, 024, 050, 052, 108, 151, 202, 497
(0.21, 0.24, 1.88)

<u>Electron Spin Resonance or Electron Paramagnetic Resonance</u>
059, 117, 120, 172, 235, 280, 338, 407, 484
(0.64, 0.49, 2.12)

<u>Extended X-Ray Absorption Fine Structure (EXAFS and XANES)</u>
023, 049, 070, 071, 072, 073, 084, 116, 125, 160, 178, 200, 255, 304
312, 313, 338, 366, 375, 410, 418, 421, 428, 432, 436, 483, 484, 493
494, 497, 506
(1.67, 1.40, 7.29)

<u>Field Emission and Field Ion Microscopy</u>
024, 190, 217, 256, 279, 358, 456, 463
(0.75, 0.49, 1.88)

<u>High Pressure (Technique development of all types)</u>
015, 047, 060, 201, 205, 245, 484
(0.31, 0.63, 1.65)

<u>Ion or Molecular Beams</u>
043, 108, 218, 222, 238, 240, 305, 324, 355, 358, 551
(0.96, 0.89, 2.59)

<u>Ion Channeling, or Ion Scattering (including Rutherford and other ion scattering methods)</u>
042, 043, 044, 045, 218, 222, 235, 238, 239, 240, 277, 302, 324, 374
391, 510
(0.94, 1.98, 3.76)

X-Ray Scattering (small angle)
040, 050, 116, 152, 160, 232, 255, 312, 418, 422, 434, 498, 507
(0.94, 0.61, 3.06)

X-Ray Scattering (other than crystallography)
017, 047, 051, 077, 160, 216, 243, 255, 360, 363, 374, 405, 416, 470
472, 474, 513, 513, 555, 559
(1.74, 1.91, 4.71)

X-Ray Photoelectron Spectroscopy
007, 016, 021, 023, 024, 049, 051, 060, 070, 081, 084, 160, 237, 262
332, 357, 359, 366, 395, 412, 418, 424, 431, 432, 450, 490, 497, 497
(1.44, 1.48, 6.59)

PHENOMENA

ENVIRONMENT

Aqueous
060, 105, 117, 121, 168, 175, 261, 262, 275, 301, 329, 337, 351, 379
395, 457, 487
(3.60, 2.63, 4.00)

Gas: Hydrogen
004, 007, 016, 073, 111, 112, 113, 144, 167, 228, 290, 291, 292, 309
354, 369, 374, 402, 441, 442, 464, 478
(4.16, 2.70, 5.18)

Gas: Oxidizing
041, 044, 148, 219, 260, 290, 292, 301, 318, 319, 339, 357, 370, 371
387, 401, 412, 441, 464
(2.66, 2.35, 4.47)

Gas: Sulphur-Containing
044, 260, 290, 292, 401, 464, 552
(0.75, 0.83, 1.65)

High Pressure
011, 015, 017, 018, 060, 075, 076, 079, 131, 166, 204, 225, 276, 323
336, 346, 418, 428, 445, 450, 458, 471, 484, 506
(3.48, 3.25, 5.65)

Magnetic Fields
008, 015, 020, 048, 049, 053, 072, 074, 075, 076, 120, 125, 157, 174
225, 226, 236, 323, 391, 392, 414, 416, 504
(2.85, 3.56, 5.41)

Radiation: Electrons
078, 122, 126, 143, 158, 263, 301, 317, 388, 435, 475
(1.51, 1.71, 2.59)

Radiation: Gamma Ray and Photons
017, 051, 053, 057, 061, 159, 192, 216, 226, 236, 317, 325, 368, 404
418, 512
(2.14, 3.10, 3.76)

Radiation: Ions
061, 218, 222, 226, 238, 239, 263, 277, 304, 321, 324, 388, 435, 481
(2.14, 3.45, 3.29)

Radiation: Neutrons
004, 056, 057, 128, 172, 200, 216, 218, 226, 236, 263, 321, 388, 410
432, 486
(1.95, 2.88, 3.76)

MAJOR FACILITIES: OPERATIONS

Pulsed Neutron Sources (Operations)
046, 203
(0.47, 4.88, 0.47)

Steady State Neutron Sources (Operations)
082
(0.24, 7.42, 0.24)

Synchrotron Radiation Sources (Operations)
083, 298
(0.47, 8.89, 0.47)

*U.S. GOVERNMENT PRINTING OFFICE:1986- 491-177:50064