DOE/ER-0581P
Dist. Category UC-404

February 1993

# Materials Sciences Programs
## Fiscal Year 1992

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences
Washington, D.C. 20585

# FOREWORD

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

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

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 1992 together with a convenient index to the Division's programs. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page.

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

# PUBLICATION REFERENCES

The Materials Sciences program has sponsored various workshops, topical and descriptive reports and co-sponsored Research Assistance Task Forces on select topics over the past 13 years. It is our intention to make as much as possible of the proceedings of these activities publically available through publication in open literature scientific journals, bulletins, or other archival forms. Many of these publications identify the authors perceptions of emerging or existing generic materials science research needs and opportunities. Their primary purpose is to stimulate creative thinking and new ideas by scientists within their respective topical fields. None of these publications, however, is intended to be all inclusive or to encompass with thoroughness any given topic, and none of them represents Department of Energy (DOE) policy or opinion. No pretense is made to have covered every materials science topic of interest in this listing, and the fact that there is no publication corresponding to a particular materials science topic does not, of itself, carry any implication whatsoever with respect to DOE interest or lack thereof. We have also included in this list the title of those publications that we anticipate will be published over the next year, so as to alert our community to this likelihood.

"Grain Boundary and Interface Phenomena in the High-Temperature Plasticity of Solids," M. E. Kassner and T. G. Langdon, editors, accepted for publication by Materials Science and Engineering, 166, 1, 1993 (23 paper dedicated issue)

"Photovoltaic Materials: Innovations and Fundamental Research Opportunities," Alex Zunger, editor, Journal of Electronic Materials, 22, 1, 1993, pp. 1-72 (8 paper dedicated issue)

"Summary Report: Computational Issues in the Mechanical Behavior of Metals and Intermetallics," M. I. Baskes, R. G. Hoagland, A. Needleman, accepted for publication by Mat. Sci. and Eng. A.

"Deformation and Fracture of Intermetallics," M. H. Yoo, S. L. Sass, C. L. Fu, M. J. Mills, D. M. Dimiduk, E. P. George, accepted for publication by Acta Metallurgica et Materialia

"Research Opportunities on Cluster and Cluster-Assembled Materials - A Department of Energy, Council on Materials Science Panel Report," R. W. Siegel, L. E. Brus, et al., J. Mater. Res., 4, 3, (1989), 704-736

"Fundamental Issues in Heteroepitaxy - A Department of Energy Council on Materials Science Panel Report," P. S. Peercy, et al., J. Mater. Res., 5, 4, (1990), 852-894

"Proceedings of the Workshop on First-Order Displacive Phase Transformations," L. E. Tanner, M. Wuttig, et al., Mat. Sci. and Eng. A, 127, 2, (1990), 137-270

"Interpenetrating Phase Composites," D. R. Clarke, J. Amer. Ceramic Soc, 75, 4 (1992) 739-759

"Hydrogen Interaction with Defects in Crystalline Solids," S. M. Myers, et al., Rev. of Modern Physics, 64 (2), April 1992, 559-617

"Proceedings of the Oak Ridge National Laboratory/Brookhaven National Laboratory Workshop on Neutron Scattering Instrumentation at High-Flux Reactors," J. D. Axe and J. B. Hayter, (1989), ORNL Report CONF-8906311

"Proceedings of the First Meeting of the International Group on Research Reactors," C. D. West, (1990), ORNL Report CONF-9002100

"Research Needs and Opportunities in Highly Conducting Electroceramics," W. J. Weber, H. L. Tuller, T. O. Mason, and A. N. Cormack, accepted for publication by Materials Science and Engineering B

"Radiation Effects on Materials in High Radiation Environments - A Workshop Summary," W. J. Weber, L. K. Mansur, F. W. Clinard, Jr., and D. M. Parkin, J. Nuclear Materials, 184, (1991), 1-21

"Welding Science: Needs and Future Directions," D. W. Keefer, S. A. David and H. B. Smartt, and K. Spence, Journal of Metals, 44, 9, 1992, 6-7

"Organic Superconductivity," (International Workshop), V. Z. Kresin and W. A. Little (eds), Plenum Press, New York, 1990, (jointly sponsored with Office of Naval Research)

"Surface, Interface, and Thin-Film Magnetism," L. M. Falicov, D. T. Pierce, et al., J. Materials Research, 5, 6, (1990), 1299-1340

"Research Needs and Opportunities in Magnetic Materials," G. Thomas, Materials Science and Engineering, B105, 3, (1990), 409-412

"Basic Research in Superconductor, Ceramic and Semiconductor Sciences at Selected Japanese Laboratories," R. J. Gottschall, DOE/ER-0410, (1989), (jointly sponsored with Office of Naval Research, U.S. Department of Commerce, and the U.S. Congress Office of Technology and Assessment)[a,b,c]

"Mechanisms and Physics of Crack Growth: Application of Life Prediction," R. B. Thompson, R. O. Ritchie, J. L. Bassani and R. H. Jones, et al., Materials Science and Engineering, A103, (1988), 1-207

"Materials Sciences in the Department of Energy," I. L. Thomas, MRS Bulletin, January 1988, 11-12

"Basic Research in Ceramic and Semiconductor Science at Selected Japanese Laboratories," R. J. Gottschall, DOE/ER-0314, (1987)[a,b]

"Molecular Monolayers and Films," J. D. Swalen, et al., Langmuir 3, (1987), 932-950

"Micromechanisms of Fracture," V. Vitek, et al., Materials Science and Engineering, 94, (1987), 5-69

"Bonding and Adhesion at Interfaces," J. R. Smith, et al., Materials Science and Engineering 83, (1986), 175-238

"Overview of DOE Ceramics Research in Basic Energy Sciences and Nonengine Energy Technology Programs," R. J. Gottschall, Ceramic Bulletin 64, (1985), 1090-1095

"Coatings and Surface Modifications," R. L. Schwoebel, et al., Materials Science and Engineering, 70, (1985), 5-87

"Novel Methods for Materials Synthesis," L. R. Testardi, T. D. Coyle, et al., (1984)[a]

"Theory and Computer Simulation of Materials Structures and Imperfections," A. B. Kunz, et al., (1984)[a]

"Materials Preparation and Characterization Capabilities," DOE/CONF-821120, February (1983)[a,b]

"Critical and Strategic Materials," R. J. Gottschall, et al., (1983)[a,b]

"High Pressure Science and Technology," G. A. Samara, et al., (1982)[a]

"Scientific Needs of the Technology of Nuclear Waste Containment," D. Turnbull, et al., (1982)[a]

"Basic Research Needs and Opportunities on Interfaces in Solar Materials," A. W. Czanderna, R. J. Gottschall, et al., Materials Science and Engineering, 53, (1982), 1-162

"The Effects of Irradiation on the Structure and Properties of Materials," C. Peter Flynn, et al., (1981)[a]

"Condensed Matter Theory and the Role and Support of Computation," J. D. Joannopoulos, A. N. Berkner, et al., (1981)[a]

"Research Opportunities in New Energy-Related Materials," J. L. Warren, T. W. Geballe, et al., Materials Science and Engineering, 50, (1981), 48-198

"Aqueous Corrosion Problems in Energy Systems," D. D. Macdonald, et al., Materials Science and Engineering, 50, (1981), 18-42

"High Temperature Corrosion in Energy Systems," R. A. Rapp, et al., Materials Science and Engineering, 50, (1981), 1-17

"Basic Research Needs on High Temperature Ceramics for Energy Applications," H. K. Bowen, et al., Materials Science and Engineering, 44, (1980), 1-56

## Description of Research Facilities, Plans, and Associated Programs

"Using Federal X-ray, Electron, and Neutron Facilities," S. Spooner, Journal of Metals, 44, 10, 1992, 72-76 and 44, 11, 1992, 67

"Scientific User Facilities, A National Resource"[a]

"Special Instrumentation Research Opportunities for Fundamental Ceramic Science at DOE," R. J. Gottschall, Ceramic Bulletin, 67, (1988), 1333-1339

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[a] Available in limited quantities from the Division of Materials Sciences by calling (301) 903-3426, -3427, or -3428

[b] Available from National Technical Information Service, U.S. Department of Commerce, Springsfield, VA 22161

[c] Available from Pro Books, Inc., P.O. Box 193, 5 Smith Street, Rockport, MA 01966 (phone: 800-783-9590 or 508-546-9590)

# INTRODUCTION

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

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

The FY 1992 funding level, title, personnel, budget activity number (e.g., 01-2) and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), Materials Chemistry (03), or Facility Operations (04). The budget numbers carry the following titles:

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

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

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

04-1 - Facility Operation

For information call (301) 903-3428 for the Metallurgy and Ceramics topics; (301) 903-3426 for the Solid State Physics and Materials Chemistry topics.

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

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

Preparation of this FY 1992 summary report was coordinated by Iran L. Thomas. Though the effort required time by every member of the Division, much of the work was done by Christie Ashton.

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# SECTION A

Laboratories

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

## AMES LABORATORY

**Iowa State University**
**Ames, IA 50011**

R. B. Thompson - (515) 294-9649
Fax No.: (515) 294-4456

**Metallurgy and Ceramics - 01 -**

O. Buck - (515) 294-4446

**1. SOLIDIFICATION MICROSTRUCTURES**
R. K. Trivedi, L. S. Chumbley, R. W. McCallum, J. D. Verhoeven
(515) 294-5869 01-1 $772,000

Studie of solidification processes and their applications to technologically important materials. Theoretical modeling of microstructural evolution and correlation between microstructures and processing conditions. Rapid solidification processing by the laser treatment of materials and by highly undercooled fine droplets. Development of microstructure/processing maps. Study of interface kinetics and the effect of crystalline anisotropy on the microstructure evolution. Directional solidification in organic materials such as succinonitrile, pivalic acid, carbontetrabromide, hexachleotyhane, t-butanol and napthalene. Directional solidification studies on segregation and morphology in gray, nodular, and white cast iron. Solidification processing of (Dy, Tb)$Fe_2$ magnetostrictive alloys, Nd-Fe-B permanent magnet materials, and intermetallic compounds, and analysis of their magnetic and mechanical properties.

**2. CONTROLLED MICROSTRUCTURES**
J. D. Verhoeven
(515) 294-9471 01-1 $234,000

Studies of processing procedures and analysis of resulting microstructures and properties. Evaluation of microstructural changes in the austempering of nodular cast irons. Study of surface characteristics of in situ Cu-refractory metal alloys. Study of magnetic properties of in situ Cu-Fe-Co alloys. Synthesis of intermetallics.

**3. MECHANICAL BEHAVIOR OF MATERIALS**
O. Buck, B. Biner, J. Kameda
(515) 294-4446 01-2 $424,000

Studies of the effects of environment and stress on the mechanical properties of metals, intermetallics, and ceramic composites. High-temperature-induced intergranular cracking in Ni base alloys. Effects of radiation-induced defects and solute segregation on intergranular embrittlement. Modeling of hydrogen embrittlement. Description of three dimensional arrays of defects and relationship of arrangement to ductility and mechanical properties. Correlation between defect structure and nondestructive measurement.

**4. MARTENSITIC PHASE TRANSFORMATIONS**
C. T. Chan, B. N. Harmon, K. M. Ho
(515) 294-7712 01-2 $134,000

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

**5. RARE EARTH AND RELATED MATERIALS**
K. A. Gschneidner, Jr.
(515) 294-7931 01-3 $367,000

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

**6. NDE MEASUREMENT TECHNIQUES**
O. Buck, D. C. Jiles, R. B. Thompson
(515) 294-4446 01-5 $364,000

Techniques to measure failure-related material properties to improve understanding of failure mechanisms and inspection reliability. Ultrasonic measurement of internal stresses, texture, and porosity. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide information about crack tip shielding and its influence on crack growth rate and detectability. Acoustic microscopy techniques for high resolution studies of microstructure and defects. Effects of fatigue damage, stress and microstructure on magnetic properties, particularly Bloch wall motion.

**7. FUNDAMENTALS OF PROCESSING OF BULK HIGH $T_c$ SUPERCONDUCTORS**
R. W. McCallum, L. S. Chumbley, J. R. Clem,
D. K. Finnemore, D. C. Johnson, M. J. Kramer
(515) 294-4736 01-5 $902,000

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

**8. ADVANCED MATERIALS AND PROCESSES**
F. A. Schmidt, I. E. Anderson,
K. A. Gschneidner, Jr., L. L. Jones,
T. A. Lograsso
(515) 294-5236 01-5 $606,000

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

**9. SCIENTIFIC AND TECHNOLOGICAL INFORMATION EXCHANGE**
F. A. Schmidt, E. O. Feinberg, T. E. Wessels
(515) 294-5236 01-5 $232,000

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

**Solid State Physics - 02 -**

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

**10. NEUTRON SCATTERING**
C. Stassis, A. Goldman, D. Vaknin, J. Zarestky
(515) 294-4224 02-1 $442,000

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

**11. NEW MATERIALS AND PHASES**
F. Borsa, R. G. Barnes, D. C. Johnston, L. Miller,
C. A. Swenson, D. R. Torgeson
(515) 294-5435 02-2 $700,000

Synthesis and characterization of new high $T_c$ superconductors and related oxides. Study of the physical properties of these new materials, such as phase equilibria and high temperature behavior. Properties of new phases including magnetic susceptibility, transport properties, heat capacity, crystallographic phase transformations, coexistence of superconductivity and magnetic order. Modeling and analysis of the data using appropriate theories. High pressure equations of state of new materials, elementary solids (ternary compounds and alloys, and alkaline earth metals), low temperature expansivity and heat capacity of materials (Lu) containing hydrogen. Applications of NMR to high $T_c$ superconductors, phase transitions, and hydrogen embrittlement of refractory metals and alloys. NMR studies of martensitic phase transformations.

**12. SUPERCONDUCTIVITY**
D. K. Finnemore, J. E. Ostenson
(515) 294-3455 02-2 $280,000

Preparation, characterization, and study of the fundamental properties of copper oxide superconductors; search for new superconducting materials; current transfer and the proximity effect near superconductor normal metal interfaces, studies of single quantized vortices for use in microprocessors and logic devices; development of superconducting composites for large scale magnets. Fundamental studies of superconductivity in metal-metal composites, use of Josephson junctions to study flux pinning of isolated vortices, development of materials with very low pinning, development of superconducting composites suitable for large scale magnets in the 8 to 16 Tesla range, practical studies to improve wire fabrication techniques, development of magnetic shielding devices.

**13. X-RAY DIFFRACTION PHYSICS**
A. Goldman
(515) 294-3585 02-2 $250,000

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

**14. OPTICAL, SPECTROSCOPIC, AND SURFACE PROPERTIES OF SOLIDS**
D. W. Lynch, C. G. Olson, M. Tringides
(515) 294-3476 02-2 $635,000

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

**15. SEMICONDUCTOR PHYSICS**
H. R. Shanks, J. Shinar
(515) 294-8706 02-2 $250,000

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

**16. SUPERCONDUCTIVITY THEORY**
J. R. Clem, V. Kogan
(515) 294-4223 02-3 $150,000

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

**17. OPTICAL AND SURFACE PHYSICS THEORY**
R. Fuchs, C. T. Chan, K.-M. Ho
(515) 294-1960 02-3 $150,000

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

**18. ELECTRONIC AND MAGNETIC PROPERTIES**
B. N. Harmon, C. T. Chan, K.-M. Ho, M. Luban, C. Soukoulis
(515) 294-7712 02-3 $492,000

Magnetic properties of new high $T_c$ superconductors. Theoretical studies of bulk and lattice dynamical properties of materials using first principles total energy calculations. Anharmonic interaction, lattice instabilities, phase transformations, electron-phonon interaction, and superconductivity. Equations of state (pressure and temperature). Hydrogen-metal interactions. Electron localization in quasi-periodic and disordered materials. Magnetism in spin glasses and ternary compounds. Electronic structure of rare earth compounds and transition metal sulfides and hydrides. Theory of amorphous semiconductors, and nuclear magnetic ordering in metals. Localization of light in dielectrics, photonics. Theoretical modeling of quantum dot nanostructures. Buckyballs.

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**Materials Chemistry - 03 -**

P. A. Thiel - (515) 294-8985

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**19. SYNTHESIS AND CHEMICAL STRUCTURE**
J. D. Corbett, J. W. Anderegg, H. F. Franzen, R. A. Jacobson, R. E. McCarley
(515) 296-3086 03-1 $760,000

Synthesis and structure of and bonding in polar intermatallic systems. Interstitial derivatives of intermetallic phases - the systematic variation of electronic, conduction, and magnetic properties and corrosion resistance. Influence of common impurities (O, N, H) on stability of intermatallic compounds. Homoatomic clusters of main-group metals in condensed phases; electronic regularities.

Synthesis, bonding, 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. Electronic band structure calculations. Study of refractory metal-rich binary and ternary sulfides and oxides 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. 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: X-ray and electron diffraction, X-ray and UV photoelectron spectroscopy, resistivity and magnetic susceptibility measurements, computer automated mass-loss-mass-spectrometry for high temperature vaporation reactions.

**20. POLYMER AND ENGINEERING CHEMISTRY**
T. J. Barton, M. Akinc, S. Ijadi-Maghsoodi, K. Woo
(515) 294-2770 03-2 $476,000

Synthesis of silicon-nitrogen polymers. Study of controlled thermal decomposition of preceramic polymers. Development of thermal and photo-chemical routes to transient compounds containing silicon-nitrogen multiple bonds as route to preceramic materials. Design and synthesis of polymers containing alternating silicon and unsaturated carbon units. Such polymers are evaluated as ceramic precursors, as electrical conductors, and as nonlinear optical materials. Synthesis and characterization of ceramic powders including oxides, sulfides and carbides. Characterization and processing of novel intermetallics for high temperature structural applications. Design and processing of ceramic matrix composites. Synthesis of new materials containing arrays of transition metal ions. Design of new monomers suited for polymerization using groups which are chosen for special photophysical or magnetic properties. Macrocyclic coordination complexes are being developed with functional side chains for the preparation of monolayers, thin films and oriented assemblies.

**21. HIGH TEMPERATURE AND SURFACE CHEMISTRY**
P. A. Thiel, K. G. Baikerikar, S. -L. Chang, R. S. Hansen, D. C. Johnson
(515) 294-8985 03-3 $485,000

Study of lubrication phenomena: decomposition pathways and products of fluorinated ethers at surfaces. Mechanisms of oxidation of metals; formation of thin, metastable oxide overlayers. 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 electron spectroscopy, electron energy loss spectroscopy, temperature programmed desorption, electron-stimulated desorption, ring-disk and modulated hydrodynamic voltammetry.

## ARGONNE NATIONAL LABORATORY

**9700 South Cass Avenue**
**Argonne, IL 60439**

F. Y. Fradin - (708) 252-3504
Fax No.: (708) 252-5888

**Metallurgy and Ceramics - 01 -**

B. D. Dunlap - (708) 252-4925

**22. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH**
N. J. Zaluzec, C. W. Allen
(708) 252-5075 01-1 $1,582,000

Development and use of high-voltage and high-spatial resolution analytical microscopy for materials research. Operation and development of the Center's 1.2 MeV High-Voltage Electron Microscope-Tandem Facility with in situ capability for direct observation of ion-solid interactions. The HVEM is currently being utilized for research programs in advanced materials, mechanical properties, irradiation effects, oxidation and hydrogenation effects. HVEM specimen stages are available for heating (1300 K), cooling (10 K), straining, resistivity and gaseous environments. Ion-beam interface with 650 kV ion accelerator and 2 MV tandem accelerator available for in situ implantations and irradiations. Approximately 50 percent of HVEM usage is by non-ANL scientists on research proposals approved by the Steering Committee for the Center that meets every 6 months. A state-of-the-art, medium-voltage, ultra-high vacuum, field-emission gun, Analytical Electron Microscope is being procured. Its design is directed toward the attainment of the highest microanalytical resolution and sensitivity. Fundamental studies of electron-solid interactions and microcharacterization of materials, using TEM, STEM, HREM, CBED, XEDS, and EELS are conducted at present on conventional transmission electron microscopes (JEOL 4000 EXII, JEOL 100CX, Philips EM420, and Philips CM30).

**23. BASIC CERAMICS**
D. J. Lam, S.-K. Chan, S. J. Rothman, J. L. Routbort, B. W. Veal
(708) 252-4966 01-3 $1,280,000

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

**24. INTERFACE STUDIES**
K. L. Merkle, J. N. Mundy
(708) 252-4990 01-3 $724,000

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

**25. IRRADIATION AND KINETIC EFFECTS**
L. E. Rehn, D. E. Alexander, R. C. Birtcher, M. A. Kirk, N. Q. Lam, P. R. Okamoto, H. Wiedersich
(708) 252-5021 01-4 $1,480,000

Investigations of mechanisms leading to the formation of defect aggregates, precipitates, and other inhomogeneous distributions of atoms in solids with and without displacement-producing irradiation. Radiation-induced segregation to internal and external defect sinks. Radiation-enhanced diffusion. Effects of irradiation on alloy composition, microstructure, grain growth, superconductivity, and amorphization. Displacement cascades, inert-gases in solids. Surface layer modification of alloys by ion implantation, ion-beam mixing, and sputtering. Ion channeling and flux-pinning in High-$T_c$ materials. Irradiation performance of advanced nuclear fuels. Effects of amorphization on dimensional stability. In situ studies of ion and electron bombardment in the High-Voltage Electron Microscope. Neutron and dual-beam ion irradiation. Computer modeling of irradiation-induced microstructural changes. Ion-beam analysis. Radiation sources include HVEM-2MV Tandem facility (electrons and ions), 650kV ion accelerator, and IPNS.

**26. HIGH $T_c$ SUPERCONDUCTOR DEVELOPMENT**
G. W. Crabtree, K. Goretta, J. L. Routbort, D. Shi
(708) 252-5509 01-5 $640,000

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

**27. AMORPHOUS AND NANOCRYSTALLINE MATERIALS**
L. E. Rehn, J. Eastman, N. Q. Lam, P. R. Okamoto, R. W. Siegel
(708) 252-5021 01-5 $658,000

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

**Solid State Physics - 02 -**

B. D. Dunlap - (708) 252-5016

**28. NEUTRON AND X-RAY SCATTERING**
J. D. Jorgensen, J. E. Epperson, G. P. Felcher, R. Kleb, R. Osborn, D. L. Price, S. Susman
(708) 252-5513 02-1 $1,600,000

Exploitation of neutron and X-ray scattering techniques in the study of the properties of condensed matter. Instrument development and interactions with university and industrial users at IPNS. Investigations of the structure and defects of intermetallic and oxide superconductors, structure and dynamics of chalcogenide and oxide glasses, liquid alloys and molten salts, surface magnetism, alloy decomposition, polymer interfaces, coarsening processes, distributions with deep inelastic scattering, and fast ion transport in solids.

**29. TWO-DIMENSIONAL MATERIALS**
S. D. Bader, M. B. Brodsky, M. Grimsditch, C. Liu
(708) 252-4960 02-2 $799,000

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

**30. SUPERCONDUCTIVITY AND MAGNETISM**
G. W. Crabtree, A. J. Fedro, K. E. Gray, D. G. Hinks, W. K. Kwok, D. J. Miller, L. C. Smedskjaer
(708) 252-5509 02-2 $1,367,000

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

**31. CERAMIC EPITAXY AND MULTILAYER STRUCTURES**
D. J. Lam, H. L. Chang
(708) 252-4966 02-2 $441,000

Coordinated experimental and theoretical research program on the processing, characterization, and property determination of epitaxial ceramic films and layered composites prepared by organometallic chemical vapor deposition techniques. Materials under investigation include: $TiO_3$, $VO_2$, $BaTiO_3$, $PbTiO_3$, $PbZrO_3$, and $PbZr_{1-x}Ti_xO_3$. A variety of experimental and theoretical techniques are used to study this problem; these include electrical conductivity and optical property measurements, conventional and high-resolution transmission electron microscopy, photoelectron spectroscopy, secondary ion mass spectroscopy, X-ray diffraction, ab initio quantum mechanical calculations and computer simulations.

**32. PHOTON SCIENCE AT SYNCHROTRONS**
P. A. Montano, M. Beno, J. C. Campuzano, G. S. Knapp, M. Ramanathan, H. You
(708) 252-6239 02-2 $552,000

Glancing incidence X-ray fluorescence has been used in the study of the elemental composition profile of superlattices. X-ray scattering techniques have been employed to study the interfacial roughness in multilayers. In-situ X-ray scattering techniques have been used to investigate the growth mode of sputtered gold on a Si single crystal as a function of temperature and rare gas pressure. The X-ray standing wave technique is being used to investigate the structure of metal/semiconductor interfaces. The group is constructing, at one the national synchrotron sources, a beam line for energy dispersive X-ray absorption measurements. Angle resolved photoemission is being employed in the characterization of the electronic properties of superconductors. The X-ray absorption technique is been used to determine the structure of excited state molecules. A new technique has been developed for rapid X-ray powder diffraction measurements.

**33. MODELING AND THEORY OF INTERFACES**
D. Wolf, S. Phillpot, S. Yip
(708) 252-5205 02-3 $265,000

Computer simulation of the physical properties of solid interfaces, such as grain and interphase boundaries, thin films and superlattices, involving atomistic simulation methods (lattice statics and dynamics, molecular dynamics, Monte-Carlo). The atomistic simulations are used to determine, for example, the structure, free energy and elastic properties of solid interfaces as a function of temperature, the point-defect properties of interfaces, such as impurity segregation and diffusion, and the properties of voids in grain boundaries and in the bulk. Materials considered involve metals, semiconductors and ceramics as well as interfaces between them.

**34. ULTRA-HIGH FIELD SUPERCONDUCTORS**
K. E. Gray, R. T. Kampwirth, D. J. Miller
(708) 252-5525 02-5 $362,000

This project includes materials engineering research and fundamental studies, both aimed at applications of superconductors, primarily in high magnetic fields. Microcharacterization has become an increasingly important part of our materials research. Studies seek to identify intrinsic limitations of crucial superconducting properties and the effect of extrinsic defects. Other studies seek to develop a low-temperature, high-rate sputtering process for high-temperature, high-field oxide superconductors (e.g., Bi-Sr-Ca-Cu-O and Tl-Ba-Ca-Cu-O), and new low-temperature in situ techniques are also being investigated. Material characterization is by X-ray, SEM, TEM, RBS, EELS, ICPAES, and superconducting properties.

**Materials Chemistry - 03 -**

D. M. Gruen - (708) 252-3513

**35. CHEMICAL AND ELECTRONIC STRUCTURE**
J. M. Williams, K. D. Carlson, U. Geiser, A. M. Kini, S. K. Kumar, J. S. Schlueter, J. Schultz, H. H. Wang
(708) 252-3464 03-1 $1,338,000

New materials synthesis and characterization focusing on synthetic organic metals and superconductors based on BEDT-TTF (bis-ethylenedithiotetrathio-fulvalene), and the fullerenes ($C_{60}$), and various new organic electron-donor and electron-acceptor molecules. Development of structure-property relationships. Electrical and superconducting properties measurements. Development of improved crystal growth techniques. Continuing development of the neutron time-of-flight single-crystal diffractometer (SCD) at the Intense Pulsed Neutron Source (IPNS). Phase transition and crystal structure studies as a function of temperature (10-300 K) using the IPNS-SCD and a low-temperature (10 K) single crystal X-ray diffraction instrument.

**36. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS**
M. Blander, L. A. Curtiss, M.-L. Saboungi
(708) 252-4548 03-2 $513,000

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

**37. INTERFACIAL MATERIALS CHEMISTRY**
V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, A. R. Krauss
(708) 252-4547 03-2 $504,000

Basic research on interfacial phenomena is being carried out in two forefront scientific fields of materials science: (1) molecular sieve materials and their application in heterogeneous catalysis and (2) novel techniques for the preparation and characterization of high-critical-temperature ($T_c$) superconductors in thin-film form. The role of organic template molecules in the crystallization mechanisms of aluminosilicate zeolites. The application of modified zeolites and metallaluminophosphate materials as catalysts in hydrocarbon oxidation reactions. Use of molecular sieve materials as matrices for the generation of interacrystalline particles and polymers, constrained in size and dimensionality. Computer simulations of framework and adsorbate molecular dynamics, as well as ab initio molecular oribital calculations of chemical properties of zeolite cataylsts and template effects in microporous structure development. Production and characterization of multicomponent thin films and layered structures by computer-controlled sequential deposition with in situ annealing and oxidation processes as part of an integrated fabrication cycle. Use of ozone atomic oxygen, and oxygen ion beam modification to produce high temperature superconductor (HTSC) films with little or no high temperature annealing. Atomic layer-by-layer fabrication of Bi based HTSCs. Production of superlattice structures for electronic applications and thin-film optoelectronic devices. Basic surface studies of as-grown superconducting thin films; basic studies of growth processes for multicomponent thin films.

**38. AQUEOUS CORROSION**
V. A. Maroni, L. A. Curtiss, C. A. Melendres, Z. Nagy, R. M. Yonco
(708) 252-4547 03-2 $611,000

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

**39. PARTICLE AND PHOTON INTERACTIONS WITH SURFACES**
D. M. Gruen, W. F. Calaway, A. R. Krauss, G. J. Lamich, M. J. Pellin, C. E. Young
(708) 252-3513 03-3 $999,000

Development of multiphoton resonance ionization methods combined with energy and angle refocusing time-of-flight mass spectroscopy for ultrasensitive detection of sputtered species. Application of this technique to studies of (1) fundamental problems in surface science (depth of origin of sputtered species; sputtering of metal clusters; adsorbate structures; strong metal support interactions; mechanisms of oxidation; surface segregation), (2) electron- and photon-induced desorption cross sections and mechanisms for neutral species with particular reference to desorption by synchrotron radiation, (3) trace analysis for selected systems of special significance such as impurities in semiconductors, (4) fundamental studies of planetary materials including isotopic anomalies. Surface composition, structure and radiation-enhanced segregation in strongly segregating alloy systems using recoil sputtering, ion-scattering, SIMS, Auger, XPS, UPS, and LEED techniques. Preparation of controlled stoichiometry high-temperature superconducting films and fabrication of layered thin-film structures by sequential sputtering of elementary targets. Ion scattering and implantation and surface modification.

**40. MOLECULAR IDENTIFICATION FOR SURFACE ANALYSIS**
D. M. Gruen, K. R. Lykke, M. J. Pellin
(708) 252-3513 03-3 $432,000

Surface analysis of the molecular composition of complex solids using Fourier transform ion cyclotron resonance spectroscopy coupled with resonant and "soft" laser ionization methods. The solid surfaces to be investigated include conducting polymers, plastics, and other high molecular weight materials. One aspect of the study involves the diffusion and fate of additives such as plasticizers and UV stabilizers in polymers. Another aspect includes the characterization of fullerene ($C_{60}$)-type compounds.

**Facility Operations - 04 -**

B. S. Brown - (708) 252-5518

**41. APS BEAMLINE AND INSERTION DEVICE R&D**
E. E. Alp, S. H. Barr, D. Carnegie, E. Gluskin, A. Khounsary, A. Macrander, D. M. Mills, E. Moog, G. K. Shenoy, D. Shu, R. K. Smither, W. Yun
(708) 252-5537 04-1 $7,365,000

Design studies of the components of the insertion devices, beamline components, X-ray optics and detectors suitable for 7-GeV Advanced Photon Source. Methodologies are developed to calculate the angular distributions and polarization of insertion device radiation and the performance of X-ray optical systems for high-brilliance photon beams. Development of a fast CCD/scintillation detector for X-ray range and readout procedures to perform time development studies are in progress. Prototype insertion devices and high heat load optics are under evaluation at the Cornell Electron Storage Ring and at the National Synchrotron Light Source X-ray ring, to assess and improve insertion device and optics performance and to conduct feasibility experimentation.

**42. APS ACCELERATOR R&D**
M. Borland, E. Crosbie, R. Damm, G. Decker, J. Galayda, G. Goeppner, J. Howell, J. Jagger, M. Knott, R. Kustom, A. Lumpkin, G. Mavrogenes, W. McDowell, D. McGhee, F. Mills, J. Noonan, A. Passi, S. Sharma, L. Teng, M. White
(708) 252-7796 04-1 $9,350,000

To further refine the accelerator and storage ring systems of the Advanced Photon Source, this research supports construction of a 7-GeV storage ring complex capable of facilitating wide ranges (1-100 kev) of X-ray tunability of insertion devices and operating with 34 insertion device beamlines. Accelerator component prototypes are developed to evaluate and refine performance characteristics. Theoretical methods are developed and applied to predict accelerator physics performance parameters. Research continues on accelerator vacuum systems fabrication and cleaning processes. Facility Title II design activities began in FY 1990, construction was initated in FY 1990 and completion is scheduled for FY 1996.

**43. INTENSE PULSED NEUTRON SOURCE PROGRAM**
B. S. Brown, F. R. Brumwell, J. M. Carpenter, R. K. Crawford, W. D. Dozier, C. -K. Loong, J. Richardson, F. J. Rotella, W. G. Ruzicka, P. Thiyagarajan, F. R. Trouw, T. G. Worlton
(708) 252-4999 04-1 $6,521,000

Operation and development of IPNS, a pulsed spallation neutron source for condensed matter research with neutron scattering techniques. The facility is equipped with 12 instruments which are regularly scheduled for users and 1 instrument under construction. 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 320 experiments, involving about 150 outside visitors from universities and other institutions are performed annually. Industrial Research on a proprietary basis, which allows the company to retain full patent rights, has been initiated with a number of companies (e.g., DuPont, Allied-Signal, IBM, General Electric, Amoco, British Petroleum) and is encouraged. Relevant Argonne research programs appear under the neutron activities of the Materials Science Division of Argonne National Laboratory.

**44. APS COMMISSIONING AND START-UP**
Y. Cho, J. Galayda, G. Shenoy
(708) 252-6616 04-1 $4,965,000

To establish a smooth transition between the construction phase and the operations phase, operations groups have been established and will grow in size until they take full responsibility for operations, maintenance and troubleshooting of all systems. Maximum use will be made of computerized documentation and document control procedures to assure repeatable, safe operations. A unified approach will be developed to create and control command sequences defining operation, associated documentation, routine maintenance record keeping and system troubleshooting. Beam stability is one of the prime measures of performance of APS. Three systems are proposed to detect three principal causes of instability in the orbit of the stored positron beam. The undulators and wigglers of APS produce the X-ray beams and are also capable of disturbing the beam stability if not adjusted to perfection. The APS staff will preview and test, among other things, the performance limits of state-of-the-art undulators. Operation of the APS relies on a long lifetime for the stored beam which depends critically on vacuum conditions. Vacuum systems and procedures will be optimized to achieve desired performance.

**45. ASD R&D IN SUPPORT OF OPERATIONS**
E. Crosbie, R. Damm, J. Galayda, M. Knott, G. Mavrogenes, L. Teng
(708) 252-7796 04-1 $1,970,000

To further develop the operations of the APS, R&D support is needed to optimize accelerator systems, control and X-ray source capabilities. These studies will examine the operating characteristics of APS systems with the goal of improving them. Activities include accelerator physics studies of the linacs, PAR, synchrotron storage ring, and transport line to increase injected currents, increase circulating current, and improve beam lifetime and stability. There is also an effort towards developing new diagnostic devices and control techniques to support accelerator physics activities and to improve integrated performance of the circulating positron beam, insertion devices and X-ray beamlines. New storage ring operating techniques are studied and devices will be developed with the goal of enhancing the ability to use the facility for synchrotron radiation research.

**46. XFD R&D IN SUPPORT OF OPERATIONS**
E. Gluskin, D. M. Mills, G. K. Shenoy
(708) 252-5537 04-1 $680,000

To prepare in advance for the operational phase of the APS facility, R&D needs have been identified that have direct bearing on the success of APS user programs. R&D items are based on user collaboration proposals, while others support the beamline design work in developing standard components. In order to enhance dissemination of the best beamline designs to the users, a Design Exchange has been established. This exchange maintains all the updated design drawings of the user beamlines from the conceptual stage to the as-built stage. Furthermore, these CAD drawings and corresponding specifications and descriptions are available to all the users on communication links. There is an additional effort to design, develop and test software to operate all the beamlines and experimental instruments so as to enhance performance and safety of operation. In addition, insertion device diagnostics will be carried out using a positron beam from the linac.

## BROOKHAVEN NATIONAL LABORATORY
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**Metallurgy and Ceramics - 01 -**

D. O. Welch - (516) 282-3517

**47. FIRST PRINCIPLES THEORY OF HIGH AND LOW TEMPERATURE PHASES**
J. W. Davenport, P. Allen (SUNY-Stony Brook), S. Narasimhan, R. E. Watson, M. Weinert
(516) 282-3789 01-1 $499,000

Molecular dynamics simulations using first principles techniques as well as empirical potentials. Applications to metals including liquids and amorphous materials. Calculations of melting and temperature dependent phase diagrams. Cluster calculations on oxide superconductors.

**48. STRUCTURE AND PROPERTIES OF SURFACE MODIFIED MATERIALS AND INTERFACES**
S. M. Heald, B. Nielsen
(516) 282-2861 01-1 $534,000

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

**49. MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS**
H. S. Isaacs, A. J. Davenport
(516) 282-4516 01-2 $441,000

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

**50. SUPERCONDUCTING MATERIALS**
M. Suenaga, R. Budhani, D. O. Welch, Y. Zhu
(516) 282-3517 01-3 $1,168,000

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

**51. BASIC MATERIALS SCIENCE OF HIGH TC CONDUCTOR FABRICATION**
M. Suenaga, Q. Li, Y. Zhu
(516) 282-3518 01-5 $657,000

The purpose of this program is to perform basic studies of problems which are associated with the fabrication of conductors for magnets and transmission of power utilizing high $T_c$ superconductors. The main focus of this program currently is on characterization of microstructural and electromagnetic properties of grain boundaries in $YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$ in order to gain increased understanding of the nature of the coupling. A second aspect of the program is the development of fabrication techniques for $YBa_2Cu_3O_7$ to strengthen the coupling of the boundaries by methods such as selective doping.

**Solid State Physics - 02 -**

M. Strongin - (516) 282-3763

**52. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES**
S. M. Shapiro, L. Passell, L. Rebelsky, B. Sternlieb, T. Thurston
(516) 282-3822 02-1 $1,433,000

This program is directed to the study of elementary excitations in condensed matter and to the development of new neutron scattering techniques to further these investigations. Currently, experimental interest focuses on excitations in heavy fermion, mixed valent, paramagnetic systems, spin glasses, magnetic alloys, and the combined use of X-rays and neutrons to study the structure and interactions in solids. Lattice dynamics studies of metallic alloys were undertaken to establish the relationship between the diffuse elastic scattering phonon anomalies in the dispersion curve. The objective in all these experiments is to obtain a better understanding of the fundamental interactions which determine the unique properties of these systems. In the area of new instrumentation, an improved reflection spectrometer has been installed on the High Flux Beam Reactor (HFBR) cold moderator beamline and is now operating. This, as well as other recently completed projects and such continuing projects as the United States-Japan (U.S.-Japan) Collaborative Research Program, represent a significant expansion of the condensed matter research capability of the HFBR. Part of the effort in new instrument development will also contribute to the Advanced Neutron Source Project at Oak Ridge National Laboratory.

**53. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS**
G. Shirane, H. Chou, P. M. Gehring, T. Thurston, J. M. Tranquada
(516) 282-3732 02-1 $1,128,000

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

**54. STRUCTURAL CHARACTERIZATION OF MATERIALS USING POWDER DIFFRACTION TECHNIQUES**
D. E. Cox, J. A. Hriljac
(516) 282-3818 02-2 $273,000

Application of synchrotron X-ray and neutron powder diffraction techniques to structural analysis of materials, including mixed metal oxides, zeolites, high $T_c$ superconductors and fullerenes. Phase transition studies at high and low temperatures, including magnetic ordering. High pressure studies in diamond--anvil cells by synchrotron X-ray diffraction techniques with monochromatic radiation. Development of instrumentation and software for powder diffraction analysis. Planning and design of a new high resolution neutron powder diffractometer. Preparation and characterization of bulk samples of inorganic materials, especially high-$T_c$ metal oxide superconductors, including $T_c$ measurements. Ab initio structure determination from powder data. Application of X-ray anomalous scattering to probe cation distribution and selective oxidation states.

**55. EXPERIMENTAL RESEARCH - X-RAY SCATTERING**
L. D. Gibbs, G. Helgesen, J. P. Hill, B. Ocko, J. Wang, G. Watson
(516) 282-4608 02-2 $1,300,000

The objective of this program is to exploit the techniques of synchrotron X-ray scattering to study the structural, electronic, and magnetic properties of condensed matter systems. The X-ray scattering group, as part of two participating research teams, operates and maintains two beamlines at the National Synchrotron Light Source (X22B and X22C) and is involved in the development and use of two new insertion device beamlines (X21 and X25). Particular emphasis is placed investigations of surface and interfacial phenomena and on the structure and magnetic spectroscopy of magnetically ordered crystals. Current examples of projects include: 1) the study of surface reconstructions and phase transformations on Au and Pt surfaces in UHV, 2) the study of electrochemically driven surface reconstructions at metal/electrolyte interfaces, 3) the study of fluctuations at liquid surfaces and interfaces, and 4) the study and use of resonant magnetic scattering in rare earths and actinide compounds.

**56. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS**
K. G. Lynn, P. Asoka-kumar, Y. Kong, P. Simpson
(516) 282-3710 02-2 $1,000,000

Perfect and imperfect solids, solid and liquid interfaces, and their surfaces are investigated by using variable energy positron (.1 eV - 3 MeV) coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron

Diffraction). These methods include two-dimensional angular correlation of annihilation radiation, positron induced Auger Electron Spectroscopy, positron channeling, positron work functions, and positronium formation. Systems that are being studied include metal-metal, oxide-semiconductor, and metal-semiconductor interfaces. Bulk positron lifetime and Doppler broadening measurements are being performed on various systems including high temperature superconductors and some metallic alloys. Defect formation in semiconductors by ion implantation and their kinetics are studied. The hydrogen interaction with the interface trap centers is studied. The early stages of pitting of aluminum have been studied. Improved modeling of positron implantation and diffusion in homogeneous and layered solids through Monte Carlo simulation is being developed to carry out quantitative depth profiling. Fundamental studies involving positron-atom scattering, single quantum annihilation, and resonant Bhabha scattering are investigated.

**57. THEORETICAL RESEARCH**
J. W. Davenport, P. Bak, V. J. Emery, Z. Olami, M. Pacuski, R. E. Watson, M. Weinert
(516) 282-3789 02-3 $882,000

Solid state theory including self organized criticality, nonlinear systems, theory of superconductivity in oxides, and many body effects. Theory of alloys including heats of formation, using local density functional theory. Electronic structure of metallic surfaces. Applications to X-ray and neutron scattering, and to photoemission.

**58. SURFACE PHYSICS RESEARCH**
M. Strongin, P. D. Johnson, P. Kuiper, M. W. Ruckman, K.-D. Tsuei
(516) 282-3763 02-5 $932,000

Various surface sensitive techniques are used to study the physical and chemical properties of surfaces and thin films. These techniques include Low Energy Electron Diffraction (LEED), Auger Electron Spectroscopy, Low Energy Ion Scattering (LEIS), Photoemission, Inverse Photoemission, and Spin Polarized Photoemission. The major part of the program is supported by beamlines at the NSLS. These include both conventional monochromators and the more advanced spherical grating monochromators used on the undulator sources. The latter devices are dedicated to the spin polarized photoemission and high resolution photoemission components of the program. Ongoing research includes: (a) photoemission and inverse photoemission studies of the electronic structure of metal overlayers, clean metal surfaces, and adsorbate covered surfaces; (b) studies of surface magnetism in thin films and the effect of adsorption on surface magnetism; (c) catalytic properties of metal overylayers; (d) photoemission and near edge studies of oxides and the high-$T_c$ superconductors; (e) surface metallurgy and surface compounds; and (f) studies of oxides and metastable species formed in low temperature reactions; (g) formation of surface coating using cryogenic techniques and synchrotron radiation.

**Materials Chemistry - 03 -**

**59. NEUTRON SCATTERING - SYNTHESIS AND STRUCTURE**
J. Z. Larese
(516) 282-4349 03-1 $473,000

A variety of neutron scattering techniques are employed to study phase transitions and critical phenomena of atomic and molecular films adsorbed on surfaces. Primary emphasis is focussed on the structure and dynamics of hydrocarbon and rare gas films adsorbed on graphite and magnesium oxide surfaces. Other areas of study include the imaging of Rayleigh-Benard convection in liquid helium mixtures, the synthesis of high-quality single-crystal materials with unique physical properties, and molecular dynamics simulations of surface films. A new Triple-Axis Multidector Powder Attachment (TAMPA) with 15 helium detectors equally distributed over a 90 degree arc allows rapid collection of powder diffraction data. A high-resolution two-dimensional neutron detector with spatial resolution <0.5 mm and a 5 x 5 $cm^2$ active area is nearly complete. Each of the new dectors provides more than an order of magnitude increase in data collection efficiency.

**60. SYNTHESIS AND STRUCTURES OF NEW CONDUCTING POLYMERS**
J. McBreen
(516) 282-4513 03-2 $487,000

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

**Facility Operations - 04 -**

M. Knotek - (516) 282-4966

**61. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS**
M. H. Brooks, W. Brynda, J. Detweiler, O. Jacobi, J. Junker, V. Lettieri, J. Petro, T. Prach, R. Reyer, D. C. Rorer, P. Tichler
(516) 282-4061    04-1  $23,506,000

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

**62. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT**
D. B. McWhan, I. Ben-Zvi, E. Blum, N. Fewell, J. Hastings, R. Heese, R. Klaffky, S. Kramer, D. P. Siddons, W. Thomlison, G. P. Williams
(516) 282-3927    04-1  $16,358,000

This program supports the operation of the National Synchrotron Light Source (NSLS), which is a large user facility devoted to the production and utilization of synchrotron radiation, and it supports the development of electron based radiation sources and new applications of this radiation in the physical and biological sciences. The NSLS operates two electron storage rings and the associated injection system composed of a linear accelerator and a booster synchrotron, and it operates an extensive user program built around facility and participating research team photon beamlines on the vacuum ultraviolet (VUV) and X-ray storage rings. As this is the first facility in the U.S. that was designed expressly for the use of synchrotron radiation, there are extensive development programs to improved the stability, reliability, and lifetime of electron beams and to develop new insertion devices which give even brighter photon beams. Equally important are programs to develop new beamline instrumentation including beamline optics, monochromators and detectors which will permit users to take full advantage of the unique research capabilities offered by the NSLS. Finally, substantial maintenance, upgrade, and safety programs are required for the operation of the facility.

## IDAHO NATIONAL ENGINEERING LABORATORY
**Idaho Falls, ID 83415**

D. W. Keefer - (208) 526-8003
Fax No.: (208) 526-5977

**Metallurgy and Ceramics - 01 -**

**63. STRESS DISTRIBUTION IN GRADED MICROSTRUCTURES**
B. H. Rabin
(208) 526-0058    01-5  $235,000

Develop fundamental understanding of the effects of microstructure, processing conditions, and specimen geometry on the residual stresses in graded materials intended to mitigate the effects of the mismatch in properties at dissimilar material interfaces. Fabrication of two-phase materials with controlled microstructural gradients and varying geometries by electron beam coevaporation and powder metallurgy techniques. Focus on materials systems in which significant property mismatch exists between components, e.g., $Al_2O_3$/Ni and Si/Ag. Measurement of residual stresses by high spatial resolution X-ray diffraction methods using synchrotron source. Comparison of experimental results with predictions from elastic-plastic finite element modeling of stress distributions.

**64. ROLE OF IMPURITIES IN MICROSTRUCTURAL EVOLUTION OF RAPIDLY SOLIDIFIED MATERIAL**
R. N. Wright
(208) 526-6127    01-5  $132,000

Examination of phenomena associated with the interaction of low levels of impurities with quenched-in defects in rapidly solidified metals. Interactions studied in simple systems to determine fundamental mechanisms. Initial studies of high-purity aluminum and aluminum doped with 1ppm lead containing ion-implanted helium have shown accelerated helium bubble growth when liquid lead precipitates are attached to bubbles. The influence of other low melting point metals with large atomic diameters, e.g., indium, on helium bubble growth will be studied. Rapidly quenched, high-purity aluminum and dilute aluminum alloys containing substitutional elements with different vacancy binding energies, as well as carbon as an interstitial impurity, will be examined. Experimental techniques include positron annihilation and TEM. Atomistic models will be developed.

## UNIVERSITY OF ILLINOIS MRL

**104 S. Goodwin Avenue**
**Urbana, IL 61801**

H. Birnbaum - (217) 333-1370
Fax No.: (217) 244-2278

**Metallurgy and Ceramics - 01 -**

H. Birnbaum - (217) 333-1370

**65. THEORY OF DEFECTS AND INTERFACES IN BCC METALS**
J. Adams
(217) 244-7709 01-1 $143,923

Theoretical calculations of defect properties in BCC systems. Development of accurate interatomic potentials. Calculation of grain boundary properties in BCC metals. Effects of H and He on properties.

**66. TRANSPORT PROCESSES IN LOCALIZED CORROSION**
R. C. Alkire
(217) 333-3640 01-1 $216,643

Corrosion of passivating systems. Tranport, 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.

**67. DEFECTS, DIFFUSION, AND NON-EQUILIBRIUM PROCESSING OF MATERIALS**
R. S. Averback
(217) 333-4302 01-1 $406,965

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

**68. MOLECULAR SPECTROSCOPY OF THE SOLID-LIQUID INTERFACE**
P. W. Bohn
(217) 333-0676 01-1 $83,763

In situ molecular spectroscopic probes used to study the structural chemistry of corrosion inhibitors on metal and metal-oxide surfaces. Raman spectroscopy of the liquid-solid interface will be used to determine absorbate-substrate binding and linear dichroism to probe the supermolecular structure and molecular orientation. Correlation with the solution chemistry and corrosion response will be made.

**69. CENTER FOR MICROANALYSIS OF MATERIALS**
J. A. Eades, H. Farrell
(217) 333-8396 01-1 $0

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.

**70. MICROANALYSIS OF DEFECTS AND INTERFACES**
J. A. Eades
(217) 333-8396 01-1 $137,742

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

**71. ATOMISTICS OF GROWTH AND TRANSPORT AT METAL AND SEMICONDUCTOR INTERFACES**
G. Ehrlich
(217) 333-6448 01-1 $156,225

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

**72. APPLICATION OF SURFACE CHEMISTRY TECHNIQUES TO UNDERSTANDING HETEROEPITAXY**
H. Farrell
(217) 333-0386 01-1 $99,293

Quantification of bulk concentration analysis using surface sensitive techniques, e.g., Auger Electron Spectroscopy and/or X-ray Photoelectron Spectroscopy, for depth profiling when differential sputtering induces surface segregation. Application of surface analysis methods to study the initial stages of heteroepitaxy at polar interfaces. Studies of structure and chemistry in the submonolayer region.

**73. SURFACE STUDIES OF BOUNDARY LAYER FILMS**
A. J. Gellman
(217) 244-5810 01-1 $42,283

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

**74. ATOMIC RESOLUTION ELECTROCHEMISTRY OF CORROSION AND DEPOSITION PROCESSES**
A. A. Gewirth
(217) 333-8329 01-1 $97,749

Scanning Tunneling Microscopy and Atomic Force Microscopy is applied to understanding the atomic processes of corrosion and deposition in electrochemical environments.

**75. TRANSMISSION ELECTRON MICROSCOPY OF SURFACES AND INTERFACES**
J. M. Gibson
(217) 333-2997 01-1 $183,030

Elucidation of surface and interface structure using quantitative transmission electron microscopy. TEM studies of surface reactions and in situ epitaxial growth using image formation using surface related diffracted intensities. Quantitative atomic resolution microscopy is being applied to interface structure and chemistry.

**76. CHEMISTRY OF NEW TRANSITION METAL CERAMIC COMPOUNDS SYNTHESIZED BY MOCVD**
G. S. Girolami
(217) 333-2729 01-1 $107,410

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

**77. CRYSTAL GROWTH AND PHYSICAL PROPERTIES OF METASTABLE SEMICONDUCTING, CERAMIC AND METALLIC ALLOYS**
J. E. Greene
(217) 333-0747 01-1 $193,656

Mechanisms and kinetics of crystal growth. Metastable single crystal alloys for solar and optical applications. Ion-beam sputtering, molecular-beam epitaxy, laser heating and low-energy ion bombardment methods applied to III-V based compounds and III-IV-V2 chalcopyrite systems.

**78. SURFACE AND INTERFACE X-RAY DIFFRACTION**
I. K. Robinson
(217) 244-2949 01-1 $54,004

Use of X-ray scattering methods to study the structure and chemistry of surfaces. Development of methods to study the structure of surfaces during MBE growth and during corrosion. Studies of the solid-liquid interface.

**79. ORGANIZATION OF THE SINGLE-CRYSTAL SOLID-LIQUID INTERFACE: ENERGIES, STRUCTURES AND ELECTRONIC SYNERGISM**
A. Wieckowski
(217) 333-7943 01-1 $144,167

Structure and properties of the solid-liquid interface. Atomic level studies of the structure/energy characteristics of adsorbates in electrochemical systems. Electrocatalysis.

**80. MICROSTRUCTURE EVOLUTION, INTERFACES AND PROPERTIES IN STRUCTURED CERAMIC COMPOSITES**
A. Zangvil
(217) 333-6829 01-1 $233,618

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

**81. SOLUTE EFFECTS ON MECHANICAL PROPERTIES OF GRAIN BOUNDARIES**
H. K. Birnbaum, I. Robertson
(217) 333-1370 01-2 $266,229

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

**82. COUNCIL ON MATERIALS SCIENCE**
C. P. Flynn
(217) 333-1370 01-2 $72,288

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.

**83. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF CERAMICS**
D. F. Socie
(217) 333-7630 01-2 $71,132

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

**84. MICROSTRUCTURE BASED CONTINUUM MODELING OF THE MECHANICAL BEHAVIOR OF MATERIALS**
P. Sofronis
(217) 333-2636 01-2 $65,184

Theoretical modeling of mechanical properties such as hydrogen interactions with dislocations, high temperature creep of nanophase materials, and sintering of ceramic compacts. Development of algorithms for describing mechanical behavior including time dependence and mass flow.

**85. SUBCRITICAL CRACK GROWTH IN STRUCTURAL CERAMICS**
J. F. Stubbins
(217) 333-6474 01-2 $83,081

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

**86. STRUCTURE AND KINETICS OF ORDERING TRANSFORMATIONS IN METAL ALLOYS AND SILICIDE THIN FILMS**
H. Chen
(217) 333-7636 01-3 $231,127

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.

**87. MATERIALS CHEMISTRY OF OXIDES CERAMICS; FIELD RESPONSIVE OGRANIC INCLUSION COMPLEXES**
W. F. Klemperer
(217) 333-2995 01-3 $343,329

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.

**88. SYNTHESIS AND PROPERTIES OF ELECTRICAL CERAMICS**
D. A. Payne
(217) 333-2937 01-3 $485,150

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

**89. ATOMIC SCALE MECHANISMS OF VAPOR PHASE CRYSTAL GROWTH**
A. Rockett
(217) 333-0417 01-3 $242,036

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

**90. PROCESSING OF MONODISPERSE CERAMIC POWDERS**
C. Zukoski
(217) 333-7379 01-3 $399,275

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.

**91. MICROSCOPIC PROCESSES IN IRRADIATED CRYSTALS**
R. S. Averback, C. P. Flynn
(217) 333-4302 01-4 $24,963

Fundamental processes of irradiation induced defects in crystalline solids. Use of high resolution analytical methods such as TEM, SIMS, RBS, to explore the atomic processes at the size scale of the defect events. Thermal spike behavior, radiation induced diffusion, radiation sputtering and sink behavior are being studied. Experimental efforts are complemented by molecular dynamic computer simulations.

**92. RADIATION EFFECTS IN METALS AND SEMICONDUCTORS**
I. M. Robertson
(217) 333-6776 01-4 $70,037

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.

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**Solid State Physics - 02 -**

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

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**93. SYNTHESIS AND CHARACTERIZATION OF ORGANOMETALLIC LIQUID CRYSTAL POLYMERS**
T. L. Brown
(217) 244-1176 02-2 $57,426

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

**94. MICROSCOPIC MECHANISMS OF CRYSTAL GROWTH**
D. Cahill
(217) 333-6753 02-2 $72,073

Development and use of microanalytic tools to study vapor phase crystal growth. Use of STM imaging combined with low energy ion energy transfer to surface atoms to study the mechanisms of growth of pure elements and alloys. Study of the effects of surface chemistry on the incorporation of adatoms into the crystal structure.

**95. ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES**
T.-C. Chiang
(217) 333-2593 02-2 $160,107

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

**96. OPTICAL AND MAGNETO-OPTICAL STUDIES OF THE ELECTRONIC STRUCTURE OF SOLIDS**
S. L. Cooper
(217) 333-2589 02-2 $51,016

Application of Fourier-transform photoluminescence, reflectivity, and ellipsometry to study the effects of impurities and dimensionality on the electronic structure of dilute magnetic semiconductor epilayers and heterostructures. Spin-flip Raman, Brillouin scattering, and Faraday rotation methods will be used to study the magnetic phase diagram of epilayers and heterostructures.

**97. GROWTH AND PROPERTIES OF NOVEL MBE MATERIALS**
C. P. Flynn
(217) 244-6297 02-2 $168,526

Determination of the mechanisms of epitaxial growth of metals and oxides. Development of a predictive framework for understanding the growth of metastable and stable structures accessible by MBE methods. Growth of multilayer systems of interest for technological applications.

**98. THEORY OF SOLIDS, SURFACES AND HETEROSTRUCTURES**
R. M. Martin
(217) 333-4229 02-2 $103,347

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

**99. SEMICONDUCTOR/INSULATOR STRUCTURES**
H. Morkoc
(217) 333-0722 02-2 $128,553

Development of novel techniques of crystal growth based on MBE, Gas Beam, and MOCVD methods. Application of methods to growth of controlled interfaces and multilayers involving semiconductors and insulators. Understanding the electronic and optical properties of these structures.

**100. DESIGN AND SYNTHESIS OF NEW ORGANOMETALLIC MATERIALS**
T. B. Rauchfuss
(217) 333-7355 02-2 $97,519

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

**101. PROPERTIES OF CRYSTALLINE AND LIQUID CONDENSED GASES**
R. O. Simmons
(217) 333-4170 02-2 $178,237

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.

**102. NUCLEAR MAGNETIC RESONANCE IN SOLIDS**
C. P. Slichter
(217) 333-3834 02-2 $202,682

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

**103. ELECTRO-ACTIVE AND NONLINEAR OPTICAL POLYMERS**
S. I. Stupp
(217) 333-4436 02-2 $234,280

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

**104. METALLOPORPHYRINS AS FIELD RESPONSIVE MATERIALS**
K. S. Suslick
(217) 333-2794 02-2 $60,735

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

**105. CARRIER TRANSPORT IN QUANTUM WELLS - PICOSECOND IMAGING**
J. P. Wolfe
(217) 333-2374 02-2 $122,937

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

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**Materials Chemistry - 03 -**

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

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**106. HIGH PRESSURE STUDIES OF MOLECULAR AND ELECTRONIC PHENOMENA**
H. G. Drickamer
(217) 333-0025 03-1 $343,000

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

**107. MECHNISTIC AND SYNTHETIC STUDIES IN CHEMICAL VAPOR DEPOSITION**
R. G. Nuzzo
(217) 244-0809 03-3 $30,765

In situ surface analysis techniques are directed towards understanding the atomic mechanisms of chemical vapor deposition growth of surface films and surface modified structures. Reactive gas-solid interactions studied with XPS, EELs, LEED and other surface methods.

**108. MICROSCOPIC THEORIES OF THE STRUCTURE AND PHASE TRANSITIONS OF POLYMERIC MATERIALS**
K. S. Schweizer
(217) 333-6440 03-3 $13,937

Development of novel molecular scale statistical mechanical theories of the equilibrium properties of polymers. Applications to the structural, thermodynamic, and phase transition behavior of polymer blends, copolymers, and melts. Development of a chemically realistic predictive theory of behavior as a design tool for synthetic chemists.

**109. OPTICAL SPECTROSCOPY OF SURFACE PROCESSES IN THIN FILM DEPOSITION**
E. G. Seebauer
(217) 333-4402 03-3 $20,266

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

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**Metallurgy and Ceramics - 01 -**

D. S. Chemla - (510) 486-4999

**110. NATIONAL CENTER FOR ELECTRON MICROSCOPY**
U. Dahmen
(510) 486-4627 01-1 $1,645,000

Organization and operation of a national, user-oriented resource for transmission electron microscopy. Maintenance, development, and application of specialized instrumentation including an Atomic Resolution Microscope 1.6A point-to-point (ARM) for ultrahigh-resolution imaging a 1.5-MeV High Voltage Electron Microscope (HVEM) with capabilities for dynamic in-situ observations, analytical electron microscopes for microchemical analysis, and support facilities for specimen preparation, image analysis, image simulation, and instrument development.

**111. CRYSTALLOGRAPHY OF MICROSTRUCTURES**
U. Dahmen
(510) 486-4627 01-1 $190,000

Investigation of fundamental features underlying the evolution of microstructures in solids by application of crystallographic techniques to the analysis of topology and defects in crystalline materials. Crystallographic relationships of precursor or parent phases and their use in analysis of defect structures and synthesis of new and unique microstructures with defect configurations reflecting composite symmetries. Electron microscopy investigation of the structure and distribution of defects such as inclusions, grain boundaries, domain walls and dislocations. Detailed characterizaton of the atomic structure of interfaces by conventional, in situ and atomic resolution microscopy in tandem with computer image simulations.

**112. ALLOY PHASE STABILITY**
D. de Fontaine
(510) 642-8177 01-1 $226,000

Calculate temperature - composition phase diagrams from first principles. Combine existing electronic band structure and total energy computational procedures with the cluster variation method (CVM) to calculate phase equilibria without empirical parameters. Phenomena of current interest are the oxygen ordering in high temperature superconductors and the prediction of long-period superstructures and anti-phase boundaries in fcc ordered substitutional alloys. Comparison with experiment is made using transmission electron microscopy and X-ray diffraction.

**113. IN SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY**
J. W. Evans
(510) 642-3807 01-1 $60,000

Microstructural aspects of gas-solid reactions. Focus of attention is porous silicon, its oxidation and identification of the oxide by viscous flow. Porous silicon is effective in reducing oxidation induced stacking faults in silicon wafter processing and a patent application has been filed. Another potential application of porous silicon in the semiconductor industry is in the formation of dielectric layers. Current practice is to form such layers by oxidation of the (dense) wafer. Oxidation of porous silicon proceeds more readily, e.g., at lower temperatures. Oxidation proceeds rapidly to form porous silica which then densified slowly. That densification is by viscous flow and the stability of cylindrical voids in a viscous medium has been examined mathematically with results published in J. of Appl. Phys. The closure of spherical voids following collapse of cylindrical voids is under examination with mathematical analysis supplemented by experiments on model pores produced by microlithography. Another part of this project concerns application of percolation theory to chemical vapor infiltration.

**114. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES**
R. Gronsky
(510) 486-5674 01-1 $159,000

Transformation interfaces: homophase boundaries, heterophase boundaries, and 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.

**115. THIN FILM STRUCTURES AND COATINGS**
K. M. Krishnan
(510) 486-4614 01-1 $100,000

The goals of this research are the synthesis and characterization of atomically-engineered thin films with novel magnetic, optical, and mechanical properties. Focus is on magnetic ultrathin multilayers and films and low-pressure deposition of diamond on ceramic substrates. Fundamental investigations of new phenomena as well as the development, control and optimization of microstructures to achieve enhanced properties will be stressed. In addition to synthesis and property measurement, development nanoscale spectroscopic, imaging and diffraction methods at the appropriate level of resolution, with either electron or photon probes, will be critical to the success of these investigations and hence will be an integral part of these research projects. Of current interest in this program are the synthesis and understanding of ultrathin magnetic nanostructures, development of a new ferromagnetic thin film with perpendicular anisotropy and potential for semiconductor-magnetic device integration, electronic structure changes associated with magnetic and chemical transitions in binary transition metal alloys and the low pressure deposition of diamond coatings on ceramic substrates. In the latter case, questions pertaining to the early stages of nucleation of diamond, the structure of the substrate/film interface and factors affecting the adhesion and surface profile of the films are being addressed.

**116. CAM HIGH PERFORMANCE METALS PROGRAM**
J. W. Morris, Jr., R. O. Ritchie, G. Thomas
(510) 486-6482 01-1 $854,000

This CAM program focuses on advanced structural metals of interest to American industry. It includes fundamental research on microstructure and mechanical behavior and specific investigations of advanced structural metals. It is organized into two projects: (1) Mechanical Behavior (R. O. Ritchie), which addresses the mechanisms of structural failure, including the fatigue and fracture in metals and intermetallics and (2) Metals (J. W. Morris, Jr.), which is concerned with the properties and development of metal alloys, including modern Al-Li alloys for aerospace applications, formable steels for manufacturing, advanced intermetallics, and materials for high field superconducting magnets. The research also includes theoretical studies of microstructure and phase transformations in metals which is integrated, as appropriate, into the other sections of the program.

**117. SOLID-STATE PHASE TRANSFORMATION MECHANISMS**
K. H. Westmacott
(510) 486-5663 01-1 $79,000

Factors that govern phase stability in order to facilitate first-principle alloy design. Advanced electron-optical techniques, especially high-voltage and high-resolution electron microscopy. The relationship between lattice defects and precipitate phase growth. Theoretical and experimental investigation of the fundamental principles underlying heteroepitaxial thin film growth.

**118. CAM CERAMIC SCIENCE PROGRAM**
L. C. DeJonghe, R. Cannon, A. Glaeser, R. Ritchie, G. Thomas
(510) 486-6138 01-3 $1,340,000

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

**119. CAM ELECTRONIC MATERIALS PROGRAM**
E. Haller, E. Bourret, W. Walukiewicz,
J. Washburn, E. Weber
(510) 486-5294 01-3 $1,166,000

Research in this program focuses on an improved understanding of the materials science of artificially structured semiconductor and semiconductor-metal systems. Basic studies concentrate on the relationships between synthesis and processing conditions and the properties of semiconductor materials, as modified by the resulting structural and electronic imperfections. Growth of compound semiconductors by metalorganic epitaxies is combined with detail studies of structural and electronic properties of thin films and interfaces. Extensive transmission electron microscopy investigations of the nature and origin of defects at interfaces and within epitaxial layers closely correlated with electrical measurements on the same specimens provide feedback to the crystal growth synthesis and processing work at Berkeley and at other National Laboratories. Optical spectroscopies ranging from the near UV to the far infrared region of the electromagnetic spectrum, electron paramagnetic resonance spectroscopy and electrical transport measurements give the complementary electronic properties. Theoretical and experimental work on the effects of atomic scale diffusion and the differences between solid solubility limits of dopants and the maximum concentration of free carriers is pursued. Novel types of processing methods including annealing under large hydrostatic pressures and with tunable synchrotron radiation, to increase the electrically active fraction of dopants, are explored. Progress in this area is applicable to the design of advanced photovoltaic energy conversion devices and of a large variety of sensors used in energy conversion processes.

**120. HIGH-TEMPERATURE REACTIONS**
A. W. Searcy
(510) 486-5900 01-3 $65,000

Sintering studies with crystalline and glassy oxides using TEM, BET, and weight-loss measurements. Surface thermodynamic theory and theory of time-independent distributions of matter in temperature gradients and theoretical studies of solid state reactions.

**Solid State Physics - 02 -**

D. S. Chemla - (510) 486-4999

**121. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE**
J. Clarke
(510) 642-3069 02-2 $214,000

DC Superconductivy Quantum Interference Devices (SQUIDs) have been 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 spectrometer is used to detect nuclear magnetic and nuclear quadrupole resonance in molecular solids at frequencies below 100kHz. Origins of low frequency magnetic noise, mechanisms of flux pinning, and distribution of flux pinning energies in high transition temperature superconductors are investigated. Novel experiments to study one-electron and single-Cooper pair effects in submicron junctions at millikelvin temperatures, including Coulomb blockade, resonant tunneling and effects of microwaves, are in progress.

**122. SURFACE, INTERFACE, AND NANOSTRUCTURE STUDIES USING SYNCHROTRON RADIATION IN COMBINATION WITH OTHER PROBES**
C. S. Fadley
(510) 486-5774 02-2 $250,000

The techniques of photoelectron diffraction and photoelectron holography have been further developed as unique probes of near-surface atomic structures. Photoelectron diffraction has been applied to a variety of systems, including metal overlayers on semiconductor (e.g., Ag on Si), surface phase transitions (e.g., saturated surface melting on Ge), and spin-polarized photoelectron diffraction from magnetic materials (e.g., high-temperature short-range order in Fe). The use of photoelectron holography for the direct determination of three-dimensional atomic images near surfaces has also been advanced for the case of adsorbates and thin overlayers, with images for S on Ni being the best determined from experimental data to date. The use of scanning tunneling microscopy as a complementary surface structure probe has also been initiated, and unique instrumentation combining photoelectron diffraction/holography and scanning tunneling microscopy on a synchrotron radiation beamline is being developed.

**123. NONLINEAR EXCITATIONS IN SOLID-STATE SYSTEMS**
C. D. Jeffries
(510) 642-3382 02-2 $142,000

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

**124. FAR-INFRARED SPECTROSCOPY**
P. L. Richards
(510) 642-3027 02-2 $197,000

Improvements in infrared technology are making possible increases in the sensitivity of many types of infrared and millimeter wave measurements. In this project, improved types of infrared sources, spectrometers, and detectors are being developed. Also, improved infrared techniques are being used to do experiments in areas of fundamental and applied infrared physics where their impact is expected to be large. Infrared experiments in progress include: measurements of the far-infrared absorptivity of the new high-$T_c$ superconductors, measurements of the infrared spectra of one-dimensional conductors, and measurements of the heat capacity of monolayers of adsorbates on metal films. Improvements in infrared technology include: development of thin-film high-$T_c$ superconducting bolometers for detecting X-ray, infrared, and microwave radiation, and development of low-$T_c$ superconducting thin-film quasiparticle detectors and mixers for near-millimeter wavelengths that approach quantum limited sensitivity.

**125. STUDIES OF THE METAL/SOLUTION INTERFACE WITH X-RAYS**
P. N. Ross
(510) 486-6226 02-2 $190,000

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

**126. FEMTOSECOND DYNAMICS IN CONDENSED MATTER**
C. V. Shank
(510) 486-5111 02-2 $290,000

The goal of this research program is to further the basic understanding of ultrafast dynamic processes in condensed matter. Research efforts are directed in two areas: development of new femtosecond optical pulse generation and measurement techniques, and application of these techniques to investigate ultrafast phenomena in condensed matter and novel material systems. In the course of this work we have developed measuremented techniques which allow us to resolve rapid events with the unprecedented time resolution of a few femtoseconds. The generation and compression of femtosecond pulses has been extended to cover the entire visible spectrum from 400 nm to 800 nm, providing the capability to investigate a large variety of important materials. Recent work has focused on ultrafast electron-hole dynamics in highly confined semiconductor structures (CdSe microcrystallites). Experimental results show clear evidence of coherent vibrational oscillations which modulate the dynamic dephasing of the optically excited electron-hole pairs on a 10 fs time scale. We have developed a novel three-pulse photon echo technique which allows us to separate the vibrational dynamics from the polarization dephasing process. This technique will have important applications for studying femtosecond processes in a variety of material systems. Preliminary results in CdSe indicate that electronic dephasing occurs on a 100 fs time scale, with significant contributions from acoustic phonon modes. In addition, we are applying femtosecond techniques to study electronic and vibrational dynamics in $C_{60}$. Relaxation processes in this material exhibit non-exponential behavior which is modulated by coherent vibrational oscillations corresponding to breathing and pinching modes of the $C_{60}$ molecule. We are currently investigating a number of mechanisms which may account for the unusual behavior we observe. These studies of ultrafast processes in solids will provide new information about the fundamental properties of materials. This knowledge will be useful for evaluating novel materials for future energy applications.

**127. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS**
Y. R. Shen
(510) 642-4856 02-2 $224,000

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

**128. CAM SURFACE SCIENCE AND CATALYSIS PROGRAM, INSTRUMENTATION**
G. A. Somorjai, J. Clarke, Y. R. Shen
(510) 642-3069 02-2 $275,000

The Surface Science and Catalysis program emphasizes atomic level surface characterization and the relationship between macroscopic chemical and mechanical properties and properties on the molecular scale. The Surface Instrumentation Project develops new surface science techniques including nonlinear optical techniques (sum frequency generation), the scanning tunneling and atomic force microscopies, Raman spectroscopy, diffuse low energy diffraction, photoelectron spectroscopy and diffraction.

**129. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS**
P. Y. Yu
(510) 642-8087 02-2 $101,000

The main objective of this project is to utilize picosecond and subpicosecond laser sources to study the ultrafast relaxation processes that occur in semiconductors. The processes under investigation include electron-phonon interactions, phonon-phonon interactions, and electron-electron interactions. The experiments involve exciting dense electron-hole plasmas in bulk or microstructures of semiconductors 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 properties of solids under high pressure.

**130. QUANTUM THEORY OF MATERIALS**
M. L. Cohen, L. M. Falicov, S. G. Louie
(510) 642-4753 02-3 $407,000

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

**131. CENTER FOR X-RAY OPTICS**
D. Attwood
(510) 642-4463 02-4 $2,061,000

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

**132. CAM HIGH-$T_c$ SUPERCONDUCTIVITY PROGRAM**
A. Zettl, P. Berdahl, J. Clarke, M. Cohen, R. Gronsky, C. Jeffries, S. Louie, N. E. Phillips, A. Portis, P. Richards, A. Stacy, E. Weber, P. Yu
(510) 642-4939 02-5 $604,000

Studies in three areas: basic science, thin films and their applications, and electron microscopy. Basic science (N. E. Phillips) activities are directed at developing an understanding of the known high-$T_c$ materials in the expectation that it will lead to other materials with superior properties. It includes theoretical work, the synthesis of new materials, growth of single crystals, and the measurement of physical properties (including magnetic susceptibility, transport properties, specific heat, isotope effects, mechanical properties, nonlinear electrodynamics, microwave absorption, terahertz spectroscopy, electron tunneling, and infrared absorption). Theoretical studies include first principles calculations and model-based interpretations of measured properties. Thin films and applications research (J. Clarke) includes fabrication and processing, investigation of physical and electrical properties, development of thin-film devices, including SQUIDS and other applications of Josephson devices, and bolometric radiation sensors. The electron microscopy research (R. Gronsky) features atomic resolution imaging of cations, which enables defects, grain boundary structure, interface epitaxy, and composition to be analyzed and related to synthesis conditions and to physical properties. The program benefits from collaborations with L. Falicov, D. deFontaine, E. Haller, L. DeJonghe, U. Kresin, D. Olander, J. Reimer, M. Rubin, R. Russo, G. Thomas, and J. Washburn.

**Materials Chemistry - 03 -**

D. S. Chemla - (510) 486-4999

**133. LOW-TEMPERATURE PROPERTIES OF MATERIALS**
N. E. Phillips
(510) 642-4855 03-1 $161,000

Measurements of low-temperature properties of materials, particularly specific heats but including electrical resistivity and magnetic susceptbility, to contribute to the general understanding of materials properties and behavior. Specific heat measurements between 5mK and 130K, at pressures to 20kbar and fields to 9T. Current emphasis is on heavy-fermion compounds, especially heavy-fermion superconductors, and high critical temperature superconductors. Related work on the temperature scale in the region below 1K where the scale is not well established.

**134. CAM ENZYMATIC SYNTHESIS OF MATERIALS PROGRAM**
M. D. Alper, M. Bednarski, H. Blanch, D. Clark, J. F. Kirsch, D. E. Koshand, Jr., B. Novak, P. G. Schultz, C. -H. Wong
(510) 486-6581 03-2 $578,000

Exploitation of the recent breakthroughs in bioorganic chemistry, molecular biology, and biochemistry to sue naturally occurring and genetically engineered enzymes in the synthesis of materials. Unusual monomers are synthesized and polymerized into novel polymers for materials applications. Enzymes are stabilized for extended lifetimes in reactors and for activity at high temperatures and in normally hostile solvents. Self assembling multifunctional molecules are synthesized and membrane-like films made for applications such as surface modification and sensor development.

**135. CAM POLYMERS AND COMPOSITES PROGRAM**
M. M. Denn, A. Chakraborty, S. Muller, B. Novak, J. Reimer, D. Theodorou
(510) 642-0176 03-2 $606,000

Development and synthesis of high performance polymeric materials. Currently the program consists of two projects: anistropic polymeric materials, and polymer/substrate interactions. Both are focused on the prediction and control of microstructure during the processing of polymeric materials. The first (M. M. Denn) looks primarily at liquid crystal polymers, using rheology, NMR, and structural theory to elucidate how orientation and stress develop during shaping. The way in which the multi-phasic nature of the polymer melts affects macroscopic orientation and orientation rates is of particular concern. The second project (D. Theordorou) emphasizes the theory of polymer conformation and stress state near a solid interface as a means of defining the influence of surface interactions on bulk orientation and stress, and hence on properties. Polymer synthesis and the development of computational methods for predicting structure development and the onset of dynamical instabilities are integral component of both project areas.

**136. ELECTROCHEMICAL PHASE BOUNDARIES**
R. H. Muller
(510) 462-6079 03-2 $25,000

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

**137. INTERFACIAL MATERIALS AND PROCESSES**
J. D. Porter
(510) 643-7236 03-2 $50,000

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

**138. ATOMIC LEVEL STUDIES OF TRIBOLOGICAL PROPERTIES OF SURFACES AND LUBRICANTS**
M. Salmeron
(510) 486-6230 03-2 $500,000

The purpose of this program is to understand the basic physical and chemical processes that govern the tribological properties of surfaces (adhesion, friction and wear) and to determine the role of surface films of lubricants in modifying these tribological properties. The atomic structure and the mechanical properties of adhesion and friction of surfaces at point contacts are studied with the Scanning Tunneling Microscopy (STM) and the Atomic Force Microscope (AFM). These techniques allow the study of the substrate atomic structure and that of the adsorbate before and after contact (microns) a Surface Force Apparatus (SFA) is used in combination with Second Harmonic and Sum Frequency Generation to study the conformation (orientation) and vibrational properties of monomolecular films in situ, during compressive and shear stresses. Studies employ simple model lubricants including atomic adsorbates (O, C, S, etc.), simple organic molecules, and long chain hydrocarbons (alkylsilanes, perfluorinated hydrocarbons) that can form self-assembled monolayers covalently bonded to various surfaces.

**139. SEMICONDUCTOR THIN FILMS USING NANOCRYSTAL PRECURSORS**
P. Alivisatos
(510) 643-7371 03-3 $90,000

Methods have been developed to prepare monodisperse, high quality, nanometer size crystallites of many common semiconductors. We are investigating the phase diagram of these nanocrystals. We find that they melt at lower temperatures than the bulk solid, and that they transform to deser phases at higher pressures than the bulk. These nanocrystals can be bound to metal surfaces using self-assembled monolayers. We are investigating the use of these surface-bound nanocrystals as low tempertuare precursors to thin films.

**140. HIGH-TEMPERATURE THERMODYNAMICS**
L. Brewer
(510) 486-5946 03-3 $80,000

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

**141. GROWTH MECHANISMS AT HETEROINTERFACES**
J. Kortright, M. Olmstead
(510) 486-5960 03-3 $500,000

This initiative focuses on the detailed study of the formation and properties of complex thin film heterostructures. Competing physical and chemical factors are studied. We combine theoretical studies with a variety of complementary, dynamic, in situ characterization techniques; we exploit unique high-resolution, ex situ characterization methods; we explore new methods of thin film formation. This program focuses on complex heterosystems in which materials on either side of the interface are widely disparate in structure or properties. Our results will help lay foundations to exploit promising materials in new technologies, such as multicomponent devices and protective coatings, by determining the role of structural, chemical, electronic and kinetic constraints in controlling thin film heterostructure growth. Systems chosen for initial study include: epitaxial heterostructures containing flourides and silicides; and growth of II-VI heterointerfaces on Pt and graphite using various techniques.

**142. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES**
D. R. Olander
(510) 642-7055 03-3 $200,000

The overall objective of this program is to chracterize 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 for light-water nuclear reactors are of principal interest. The processes and properties studied include rapid transient vaporization of fuel materials by laser pulsing, high temperature reactions of $UO_2$ with steam, and the release of volatile fission produce from irradiated $UO_2$. Molecular beam studies of the chemical kinetics of gas-solid reactions include hydrogen-atom and halogen reactions with silicon carbide.

**143. NUCLEAR MAGNETIC RESONANCE**
A. Pines
(510) 486-6097 03-3 $800,000

The Nuclear Magnetic Resonance (NMR) program has two complementary directions. The first is the development of new concepts and techniques in NMR in order to extend its applicability to a wide range of problems and materials. Such as undertaking involves the development of new theoretical approaches and experimental methods. Some developments currently underway in this direction are iterative pulse sequences, geometric phase, multiple-quantum NMR, zoer-field NMR, double-rotation NMR of quadrupolar nuclei, NMR imaging of density and flow, optical pumping and surface-enhanced NMR. The second direction involves the application of novel NMR methods and instrumentation to materials research. For example, the developments above are being used to study clusters and nanostructures, oxides, silicates, zerolites, aluminophsphates, catalysts, liquid crystals, polymers, icosahedral materials and glasses.

**144. CAM SURFACE SCIENCE AND CATALYSIS PROGRAM**
G. A. Somorjai, A. T. Bell, S. G. Louie, M. B. Salmeron, Y. R. Shen, M. A. Van Hove
(510) 642-4053 03-3 $1,092,000

The Surface Science and Catalysis program emphasizes atomic level surface characterization and the relationship between macroscopic chemical and mechanical properties and properties on the molecular scale. The Surface Science effort includes studies of atomic scale surface structure of solids and absorbed monolayers; the chemical (bonding reactivity) and mechanical (adhesion, friction, lubrication) properties are investigated. Hard coatings, oxide films and oxide-metal, metal-metal, and metal-polymer interfaces are prepared by vapor, plasma or sputter deposition. Catalysis research is focused on correlating macroscopic catalytic properties of microporous crystalline materials and model single crystal surfaces with their atomic surface structure, chemical bonding and composition. The catalytic materials investigated include transition metals, zeolites and other oxides, sulfides and carbides. The roles of additives that are surface structure or bonding modifiers are explored. Catalyzed reactions of interest include selective hydrocarbon conversion to produce clean fuels, nitrogen oxide reduction, hydrogenation and methanol synthesis.

**145. SYNTHESIS OF NOVEL SOLIDS**
A. M. Stacy
(510) 642-3450 03-3 $167,000

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

**146. STIMULATED DESORPTION OF HALOGENS**
J. A. Yarmoff
(714) 787-5336 03-3 $50,000

This interaction of radiation with surfaces is studied via desorption induced by electronic transitions, or DIET techniques. Of particular interest are the types of chemical systems that are important in the processing of semiconductor devices. Synchrotron radiation-based techniques are employed, including soft X-ray photoemission and photon stimulated desorption, at the National Synchrotron Light Source, Brookhaven National Laboratory, and at MAXLAB in Lund, Sweden. A number of halogen-semiconductor systems have been investigated, including $XeF_2$/Si, $XeF_2$/GaAs, $Cl_2$/GaAs, $I_2$/Si, and $I_2$/GaAs. From the $XeF_2$/Si work, a model of the halogent etching process of semiconductor surfaces has been developed. In the laboratory at the University of California, Riverside, a system to be used for studies of radiation induced surface damage via electron stimulated desorption has been constructed. In addition, when the Advanced Light Source at Lawrence Berkeley Laboratory becomes operational, it will be employed for DIET studies.

**Facility Operations - 04 -**

**147. 1-2 GEV SYNCHROTRON LIGHT SOURCE R&D**
J. N. Marx
(510) 486-5244 04-1 $10,481,000

The Advanced Light Source (ALS), now undergoing construction and preoperations activities, will provide beams of ultraviolet light and soft X-rays of unprecedented brightness. This national user facility will achieve this brightnesss through a combination of long magnetic insertion devices (undulators and wigglers) and an ultralow-emittance electron beam in a 1-2 GeV storage ring. Accelerator preoperations activities include commissioning, with beam, of the injection complex and the storage ring; putting the control system into operation; surveying and aligning all accelerator systems; and testing of beam-monitoring and feedback instrumentation. Experimental-systems preoperations activities include testing completed in sertion devices, and beam line components, developing magnet-measuring systems, designing and testing on accelerator diagnostics beam line, and establishing an optical metrology laboratory. Quality assurance and environment, health, and safety protection figure importantly in these activities. Establishment of a broad multi-disciplinary scientific program focusing on exploitation of the unique properties of the ALS also continued.

## LAWRENCE LIVERMORE NATIONAL LABORATORY

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**Metallurgy and Ceramics - 01 -**

**148. SYSTEMATICS OF PHASE TRANSFORMATIONS IN METALLIC ALLOYS**
L. Tanner
(510) 423-2653 01-1 $537,000

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

**149. EFFECT OF IMPURITIES, FLAWS AND INCLUSIONS ON ADHESION AND BONDING AT INTERNAL INTERFACES**
W. E. King, G. Campbell, S. M. Folles, A. Gonis, E. Sowa, W. G. Wolfer
(510) 423-6547 01-2 $520,000

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

**Solid State Physics - 02 -**

**150. SCIENCE OF THIN FILMS AND CLUSTERS**
L. L Chase, A. V. Hamza, J. G. Tobin
(510) 422-6151 02-2 $454,000

The electronic and geometric structures of surfaces, interfaces and ultrathin films constructed from nanocyrstalline clusters are investigated. A combination of unique synthesis methods and powerful characterization techniques are used to study nanoscale properties, such as quantum confinement, and to address issues like grain boundary effects and structure-property relationships in nanophase systems. Wet-chemical methods are used for synthesis. Characterization methods include photoelectron spectroscopies, EXAFS, X-ray diffraction, scanning tunneling and force microscopy, TEM, and small angle electron scattering. The evolution of properties as a function of particle size from the nanoscopic to macroscopic scale will be used to develop a strategy for the preparation and utilization of novel assemblies of clusters. In other investigations, the effects of energy-selective, nonthermal, electronic excitation of substrate or coating material on overlayer growth and morphology are explored. Optical and synchrotron sources are used to excite valence, core, and surface states, and surface analytical techniques are employed to characterize the resulting changes in coating or surface layer properties. A basic understanding of the mechanisms whereby overlayer growth can be controlled or modified by selective nonthermal excitation is sought. Materials and processes studied include oxidation of Si and other semiconductors, deposition of insulating or semiconducting thin films, and ion-implanted layers.

**151. OPTICAL MATERIALS RESEARCH**
S. A. Payne, C. Marshall
(510) 423-0570 02-2 $300,000

Linear and nonlinear optical properties of optical materials are investigated including: behavior of bulk properties at high laser intensities. Properties measured and modelled include absorption and emission spectra and cross sections, lifetimes of optical excitations, and nonlinear transmission and propagation effects. Coherence properties of optical excitation and ultra-high intensity behavior of materials are investigated with subpicosecond time resolution. Spectroscopic properties of laser ions in crystals and glasses are investigated using linear and nonlinear spectroscopic techniques. In support of this work new optical materials are prepared and characterized.

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**Metallurgy and Ceramics - 01 -**

D. M. Parkin - (505) 667-8455

### 152. NEUTRON IRRADIATION INDUCED METASTABLE STRUCTURES

K. E. Sickafus, Jr. Clinard, F. W., M. Nastasi
(505) 665-3457 01-4 $556,000

Irradiation phenomena and damage microstructures resulting from neutron irradiation of ceramics and intermetallic compounds. Investigation of cascade damage events in model materials, complemented by physical property measurements and ion irradiation tests, where the latter can elucidate neutron damage effects. Computer simulation is used to assist in understanding the nature of damage events.

### 153. SYNTHESIS AND PROCESSING OF SINGLE CRYSTAL SAPPHIRE FILAMENTS

W. R. Blumenthal
(505) 667-0986 01-5 $25,000

The goal of this project is two-fold and uses a multiple disciplinary approach to study single crystal sapphire filaments for potential use as high temperature creep resistant composite reinforcements. One objective is to empirically relate growth parameters used to control the Edge-defined Film-growth (EGF) and the Laser-heated Floating Zone processes to resulting microstructures and mechanical properties. A more challenging objective is to model the EFG process in order to not only optimize growth conditions for sapphire, but also for other candiate reinforcement oxides (e.g.,YAG). Microstructural and mechanical property characterization meachanisms controlling filament strength.

### 154. INTERFACIAL EFFECTS IN STRUCTURAL CERAMICS

T. E. Mitchell, A. L. Graham, J. J. Petrovic, K. E. Sickafus
(505) 667-0938 01-5 $338,000

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

### 155. MECHANICAL BEHAVIOR OF VERY HIGH TEMPERATURE STRUCTURAL CERAMICS

T. E. Mitchell, U. F. Kocks, J. J. Petrovic, D. S. Phillips, M. G. Stout
(505) 667-0938 01-5 $265,000

The purpose of this research program is to develop a fundamental understanding of the deformation behavior of ceramics at very high temperatures (greater than about <1500°C). The emphasis will be on ceramic oxides with high melting temperatures. Examples include garnets, perovskites and spinels. Single crystals and polycrystals will be deformed at high temperatures in order to quantify the kinetics of deformation and identify and characterize deformation modes, including slip systems and twinning systems. A further goal is to develop an understanding of strengthening mechanisms at high temperatures by such processes as solution hardening, second phase hardening and reinforcing with aligned eutectics. The fracture characterization of these structural ceramic materials will also be studied.

### 156. METASTABLE PHASES AND MICROSTRUCTURES

R. B. Schwarz, T. E. Mitchell
(505) 667-8454 01-5 $255,000

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

### 157. MECHANICAL PROPERTIES

M. G. Stout, U. F. Kocks, A. D. Rollett
(505) 667-4665 01-5 $546,000

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes, Bauschinger effects. Characteristics of mechanisms controlling the large strain deformation of aluminum, nickel, iron, copper, brass, tantalum, zirconium and titanium. Sub-structural and textural evolution with strain, strain-state, and strain-rate. Predictions of texture evolution using crystal plasticity and strain-rate sensitivity. Kinetics of plastic flow at room and elevated temperatures. Phenomenlogy and mechanisms of dynamic and static recrystallization. Alumina/niobium interface fracture. Measurements of mixed mode fracture energies of homogeneous materials and interfaces between material couples. Fractographic and analytic analysis of interface fracture.

**Solid State Physics - 02 -**

D. M. Parkin - (505) 667-8455

158. CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY
R. Pynn
(505) 667-6069 02-1 $2,054,000

Research in condensed-matter science using the pulsed spallation neutron source (LANSCE) at Los Alamos National Laboratory. Topics of current interest include the structure of polymers, polymer blends, colloids and other macromolecular systems in the bulk and at surfaces and interfaces, the vibration spectra of adsorbed species and hydrogen in metals, atomic arrangements of high-temperature superconductors, actinides and metal hydrides, crystallography at high pressures, texture and preferred orientation in metallurgical and geological samples, and residual stress in engineering components. Extensive collaborations are in place with researchers working on other programs at Los Alamos, as well as with staff at various outside institutions. These interactions cover a broad range of applications of neutron scattering to materials science, chemical physics, crystallography and structural biology.

**159. CORRELATED ELECTRONS IN METALS**
Z. Fisk, J. L. Smith, J. D. Thompson
(505) 665-0892 02-2 $257,000

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

**160. ULTRA-HIGH PRESSURE STUDIES**
D. Schiferl, R. LeSar
(505) 665-3150 02-2 $240,000

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

**161. PHOTOELECTRON SPECTROSCOPY OF TRANSURANICS UTILIZING A TUNABLE ULTRAVIOLET LABORATORY LIGHT SOURCE**
A. J. Arko, R. J. Bartlett, J. J. Joyce, D. D. Koelling, J. Lawrence, M. Norman, P. Riseborough
(505) 665-0758 02-5 $250,000

We will use photoelectron spectroscopy, with photons from the new laser-plasma tunable light source, for exploring the electronic structure of the 5f electrons in the actinide series; including an investigation of the localization-delocalization mechanism for f-electrons. The transition to localized f-states for the actinides will be microscopically probed and correlated with parameters such as Coulomb correlation energy, band width, hybridization strength, dispersion, anisotropy, and lifetimes; which are readily obtained from photoemission data. Emphasis will be placed on heavy Fermion compounds forming the boundary between localized and band states. The ultraviolet laboratory light source has tunability in the VUV range (30 eV to 200 eV) allowing full use of the powerful resonance photoemission technique to separate out the 5f as well as other orbital features in the spectra. The unique time structure of the laser pulses allows the utilization of pump and probe experiments to study empty 5f states just above the Fermi energy and fully complement the standard photoemission investigation of filled states.

**162. HIGH TEMPERATURE SUPERCONDUCTIVITY**
Z. Fisk, A. Arko, P. C. Hammel, I. Raistrick,
J. D. Thompson
(505) 665-0892 02-5 $673,000

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

**163. THERMAL PHYSICS**
G. W. Swift, R. E. Ecke
(505) 665-0640 02-5 $300,000

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

**Materials Chemistry - 03 -**

D. M. Parkin - (505) 667-8455

**164. INTEGRATED MODELING OF NOVEL MATERIALS**
K. S. Bedell, A. R. Bishop, A. F. Voter
(505) 667-6491 03-0 $400,000

This is a core program in condensed matter and materials theory aimed at extending the theory base available for modelling novel electoronic and structural materials. Such an integrated theory base is essential to the challenges of controlling and utilizing the unusual properties of such materials for applications in device and other technologies. A combination of techniques are represented, drawn from solid state and many body physics and quantum chemistry, including state-of-the-art analytical and numerical approaches. This theoretical technology base is used to develop new techniques and to couple them with integrated synthesis-characterization-modelling programs at Los Alamos and elsewhere. The modelling is aimed at both the basic electronic structure of strongly correlated materials, and the development of interatomic potentials for directionally bonded materials.

**165. ORIGINATING SUPER-STRONG LIQUID-CRYSTALLINE POLYMERS**
B. C. Benicewicz
(505) 665-0101 03-2 $160,000

This is a basic research project to originate the next generation of liquid-crystalline polymers (LCPs)--i.e., an entirely new class of LCPs whose strength characteristics are exceptionally superior both in magnitude and dimensionality to present LCPs. Super-strong LCPs are designed to have exceptional strength in three dimensions on a microscopic, molecular level in order to make the first super-strong LCP fibers, thin films, and bulk materials. Progress has been made in the chemical synthesis of these new LCPs, and the preparation for their experimental characterization.

**166. LOW-DIMENSIONAL MIXED-VALENCE SOLIDS**
B. I. Swanson, A. R. Bishop
(505) 667-5814 03-2 $308,000

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

**Facility Operations - 04 -**

**167. LANSCE OPERATIONS SUPPORT, SPECTROMETER DEVELOPMENT, AND USER SUPPORT**
R. Pynn
(505) 667-6069 04-1 $5,774,000

Neutron beams for condensed matter research at LANSCE are produced when a pulsed, 800 MeV beam of protons impinges on a tungsten target. The proton beam is accelerated to 800 MeV by the Los Alamos Meson Physics Facility (LAMPF) linac and its time-structure is tailored by a Proton Storage Ring (PSR) whose operation is partially supported by the Office of Basic Energy Sciences. Most of the neutrons produced by proton spallation in the LANSCE tungsten target have too high an energy to be useful for condensed matter research. To produce neutron beams of suitable energies, four moderators- three using chilled water and one using liquid hydrogen - surround the target assembly. The intense neutron beams produced by the LANSCE target-moderator assembly provides higher instantaneous data rates than have ever been experienced before at a similar installation. To facilitate the acquisition of neutron scattering data at such an intense source, a new generation of ultra-fast, computer-based modules has been developed using the international standard FASTBUS framework. Suitable neutron scattering spectrometers make optimum use of the source characteristics provided by the PSR and the advanced target-moderator system. During the next three to four years, several new spectrometers will be installed at LANSCE: the first phase of a chopper spectrometer for inelastic scattering is almost complete, while a back-scattering machine awaits the installation of a suitable neutron guide. The specrometers at LANSCE are used by researchers from government laboratories, academia and industry. Such a national user program requires LANSCE support personnel to assist in the operation of spectrometers and to familiarize users with the safe operation of the facility. A scientific coordination and liaison office has been established with the responsbility for dissemination of information about LANSCE and coordination of the user program.

## NATIONAL RENEWABLE ENERGY LABORATORY

**1617 Cole Boulevard**
**Golden, CO 80401**

R. A. Stokes - (303) 231-7625
Fax No.: (303) 231-1997

**Metallurgy and Ceramics - 01 -**

S. K. Deb - (303) 231-1105

**168. GROWTH AND PROPERTIES OF NOVEL ORDERED II-VI AND III-V SEMICONDUCTOR ALLOYS**
A. Mascarenhas, J. Olson, A. Zunger
(303) 231-1368 01-1 $500,000

The primary focus of this project is a combined experimental-theoretical effort aimed at understanding spontaneous long-range order in isovalent III-V/III-V and II-VI/II-VI semiconductor alloys. It includes (i) MOCVD growth of III-V alloys such as GaP/InP, AlP/GaP, AlP/InP, AlAs/InAs, and GaAs/GaP, (ii) MBE growth of III-VI alloys such as ZnTe/MnTe, ZnTe/CdTe, and ZnSe/ZnTe (Professor J. Furdyna, Notre Dame), (iii) Raman, modulation reflectance and photoluminescence studies of ordering in the above systems, and (iv) first-principles theoretical studies of surface-induced, epitaxially-induced and bulk ordering in these systems.

**Solid State Physics - 02 -**

S. K. Deb - (303) 231-1105

**169. SEMICONDUCTOR THEORY**
A. Zunger
(303) 231-1172 02-3 $208,000

First-principles band structure, total energy, and statistical mechanical (cluster variation and Monte-Carlo) methods are used to predict electronic and structural properties of bulk and epitaxial semiconductors superlattices, surfaces and alloys emphasizing chemical trends and properties of new materials. Current work includes (1) first-principles prediction of alloy thermodynamic quantitites (e.g., phase-diagrams) for bulk $A_xB_{1-x}C$ semiconductor alloys including order/disorder transitions, miscibility gaps, and ordered stoichiometric compounds. These methods are also applied to metallic cases, e.g., CuPd, CuAu, CuPt; (2) spontaneous ordering in ternary compounds (e.g., $(GaAs)_m$, $(GaSb)_n$ or HgTe/CdTe superlattices); (3) calculation of valence band offsets between II-VI and III-V semiconductors; (4) prediction of properties of unusual ternary materials, e.g., ordered vacancy $A^{II}B_2^{III}C_4^{IV}$ compounds (e.g., $CdIn_2Se_4$), (5) order-disorder transitions in ternary chalcopyrites (e.g., $CuInSe_2$ and magnetic semiconductors (e.g., MnTe); (6) Surface calculations for semiconductor alloys; (7) Predictions of band gaps of quantum wires, films, and boxes. Theoretical tools include (a) the total energy non-local pseudopotential method, (b) the all-electron Mixed Basis Potential Variation band structure method, (c) the total energy full-potential linearized augmented plane wave (LAPW) method, (d) the cluster variation approach to the Ising program, applied to binary and pseudobinary phase diagrams, and (e) Monte-Carlo and simulated-annealing calculations of Ising models derived from first-principles.

## OAK RIDGE ASSOCIATED UNIVERSITIES
## Oak Ridge, TN 37831

A. Wohlpart - (615) 576-4427
Fax No.: (615) 576-0202

**Metallurgy and Ceramics - 01 -**

**170. SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)**
N. D. Evans, E. A. Kenik
(615) 576-4427 01-1 $133,000

Microanalysis facilities within the Metals and Ceramics Division of Oak Ridge National Laboratory (ORNL) are available for collaborations in materials science between researchers at universities, industry, or other government laboratories and ORNL staff members. Facilities are available for state-of-the-art analytical transmission electron microscopy, scanning electron microscopy, atom probe/field ion microscopy, irradiation studies, ion beam treatments, nuclear microanalysis, and mechanical properties measurements at high spatial resolution. Analytical electron microscopy capabilities include energy dispersive X-ray spectroscopy (EDXS), parallel-detection electron energy loss spectroscopy (PEELS), and convergent beam electron diffraction (CBED). High resolution electron microscopy, low temperature (100 K), high temperature (1500 K), in situ deformation, and video recording facilities are available. Surface analysis facilities include three Auger electron spectroscopy (AES) systems and three (0.4, 2.5, and 5.0 MV) Van de Graaff accelerators for Rutherford backscattering and nuclear reaction techniques. A mechanical properties microprobed (Nanoindenter), having high lateral (0.3 μm) and depth (0.16 nm) resolution, can characterize elastic/plastic behavior in thin films, layers, interfaces, and other sub-micron features.

**171. OAK RIDGE SYNCHROTRON ORGANIZATION FOR ADVANCED RESEARCH**
P. Zschack, S. Moss, C. J. Sparks, Jr.
(516) 282-5614 01-1 $120,000

A synchrotron radiation beam line installed by the Oak Ridge National Laboratory at the National Synchrotron Light Source at Brookhaven is made available to interested users from university, industrial, and government laboratories. University staff and industrial scientists are invited to join in collaborative research in materials science of importance to DOE programs at an intense X-ray research facility not available at their home institutions. More than forty scientists annually participate in experiments at this facility. The beam line provides focused X-radiation spanning the energy spectrum from 3 to 40 keV at an energy resolution of delta E/E = $2 \times 10^{-4}$. One Oak Ridge Institute for Science and Education staff member is stationed at the NSLS to interface with the users and to assist in their experiments. Research capabilities include 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; interface studies; X-ray spectroscopy of electron rearrangements; magnetic X-ray scattering; and inelastic X-ray scattering.

## OAK RIDGE NATIONAL LABORATORY
**P. O. Box 2008**
**Oak Ridge, TN 37831-6117**

B. R. Appleton - (615) 574-4321
Fax No.: (615) 574-0323

**Metallurgy and Ceramics - 01 -**

L. L. Horton - (615) 574-5081

**172. MICROSCOPY AND MICROANALYSIS**
J. Bentley, E. A. Kenik, M. K. Miller, W. C. Oliver
(615) 574-5067 01-1 $1,068,000

Development and application of analytical electron microscopy (AEM), atom-probe field-ion microscopy (APFIM), and mechanical properties microprobes (MPM) to determine the microstructure, microchemistry and mechanical properties of materials at high spatial resolution. Maintenance of SHaRE User facilities and collaborative research with non-ORNL users. Equilibrium and radiation-induced segregation at grain boundaries and interfaces by APFIM/AEM, correlation of GB structure and segregation. Applications of advanced EDS, EELS, and reflection electron microscopy techniques.

inelastic electron scattering. APFIM characterization of intermetallics, spinodals, early stages of phase transformations, and irradiated pressure vessel steels. Structural ceramics, ion-implanted ceramics, intermetallics.

**173. THEORETICAL STUDIES OF METALS AND ALLOYS**
W. H. Butler, C. L. Fu, G. S. Painter, G. M. Stocks
(615) 574-4845 01-1 $967,000

Use of density functional theory and other techniques to calculate the properties of materials. Development of new techniques for calculating properties of materials. Use of KKR-CPA to calculate such properties of alloys as phase diagrams, thermodynamic properties, magnetic properties, lattice constants, short-range order parameters, electrical and thermal resistivities. Use of high-speed band theory (FLAPW, pseudopotential, LMTO, QKKR) to calculate total energies of metals and intermetallic compounds. Calculation of the elastic constants, and the energetics of planar and point defects of metals and intermetallic alloys, and the use of these quantitites to understand their mechanical properties. Use of density functional thoery 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.

**174. X-RAY RESEARCH USING SYNCHROTRON RADIATION**
C. J. Sparks, Jr., G. E. Ice, E. D. Specht
(615) 574-6996 01-1 $444,000

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

**175. RADIATION EFFECTS**
L. K. Mansur, W. R. Allen, K. Farrell, E. H. Lee, M. B. Lewis, R. E. Stoller
(615) 574-4797 01-4 $1,532,000

Theoretical and experimental research on defects and microstructures produced by irradiation, by ion beam treatment and by related processes. Principles for design of improved materials. Studies using multiple simultaneous ion beams. Ion beam modification of phase relationships and surface-sensitive mechanical properties of metallic and polymeric materials; new materials by ion beam processing. Neutron damage in metals and alloys irradiated in HFIR, FFTF and other reactors. Effect of alloying additions; effect of energy spectrum and damage rate; radiation-induced embrittlement, creep and swelling; phase stability under irradiation; relationship between ion and neutron damage; effect of helium and other impurities on microstructure and microcomposition; helium diffusion and lattice site location; theory of microstructural evolution based on defect reactions; Fe, Al, Zr, Ni, and austenitic Fe-Cr-Ni alloys; ferritic alloys; MgO, $Al_2O_3$, $MgAl_2O_4$.

**176. MICROSTRUCTURAL DESIGN OF STRUCTURAL CERAMICS**
P. F. Becher, K. B. Alexander, A. Bleier, C.-H. Hsueh
(615) 574-5157 01-5 $1,037,000

Experimental and theoretical approaches are being developed to provide new insights into mechanisms which improve the toughness, strength, and elevated temperature mechanical performance of ceramics with companion studies in ceramic processing leading to controlled densification, microstructures and compositions, in such toughened systems. The pertinent micro- and macro-scopic characteristics are directly related to phenomena that are controlled during powder synthesis, powder processing, and densification. Thus, this task incorporates interdisciplinary studies of the fundamental descriptions of powder processing and its 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 creep mechanisms. A primary consideration of these studies is providing the fundamental insights for design and fabrication of ceramics and ceramic composites for elevated temperatures.

**177. FUNDAMENTALS OF WELDING AND JOINING**
S. A. David, J. M. Vitek, T. Zacharia
(615) 574-4804 01-5 $489,000

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

**178. HIGH TEMPERATURE ALLOY DESIGN**
C. T. Liu, E. P. George, J. A. Horton,
C. G. McKamey, J. H. Schneibel, M. H. Yoo
(615) 574-4459 01-5 $1,268,000

Design of ordered intermetallic alloys based on $Ni_3Al$ FeAl, NiAl, $MoSi_2$, and other aluminides (e.g., $TiAl_3$). Study of the effect of alloy stoichiometry on structure and properties of grain boundaries, nature and effects of point defects, and microalloying and grain-boundary segregation. Study of superlattice dislocation structure, solid-solution hardening, mechanistic modeling of anomalous temperature dependence of yield stress, impact resistance and crack growth, and deformation and fracture behavior of aluminides in controlled environments at ambient and elevated temperatures. Study of superplastic behavior, grain-boundary cavitation, and theoretical modeling of creep behavior of $Ni_3Al$ alloys. Study of the effect of electron structure and atomic bonding on both intergranular and transgranular fracture (e.g., cleavage). Experimental work on structure and properties of aluminide materials prepared by conventional methods and innovative processing techniques. Establishment of correlation between mechanical properties, microstructural features, and defect structures in aluminides. Study of processing parameters on reaction kinetics and microstructural evolution of aluminides processed by reaction synthesis (combustion synthesis).

**Solid State Physics - 02 -**

J. B. Roberto - (615) 574-6151

**179. STRUCTURES OF ANISOTROPIC COLLOIDAL MATERIALS**
J. B. Hayter, W. A. Hamilton
(615) 576-9300 02-1 $495,000

Small-angle neutron scattering and neutron reflectometry studies of colloidal systems. Objectives of this research are to determine how structural features initially present in liquid-phase colloidal dispersions are preserved or modified as these systems are processed to form nanoscale materials. A major goal is to understand the role of colloidal anisotropy in determining final structures. In collaboration with L. Magid, University of Tennessee, and R. Pynn, LANL.

**180. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS**
R. M. Moon, J. W. Cable, J. Fernandez-Baca,
H. A. Mook, R. M. Nicklow, H. G. Smith
(615) 574-5234 02-1 $1,000,000

Inelastic neutron scattering studies of phonons, magnons, and single-particle excitations in condensed matter, elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials, lattice dynamics, magnetic excitations in amorphous systems, phase transitions, nuclear spin ordering, momentum distributions in quantum fluids. New research directions will include more emphasis on materials properties under extreme environments of high pressures, high temperatures, or ultralow temperatures.

**181. STRUCTURE AND DYNAMICS OF ENERGY-RELATED MATERIALS**
R. M. Moon, H. R. Child, H. A. Mook, S. Spooner,
G. D. Wignall
(615) 574-5234 02-1 $1,360,000

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

**182. PROPERTIES OF ADVANCED CERAMICS**
J. B. Bates, N. J. Dudney, G. R. Gruzalski,
D. C. Lubben, F. A. Modine
(615) 574-6280 02-2 $562,000

Physical and chemical properties of advanced ceramics including single-phase thin-film, layered, and surface-modified structures prepared by novel techniques. Materials investigated include, thin films of amorphous and crystalline metal oxides and oxynitride ionic and mixed ionic-electronic conductors. Films prepared by magnetron sputtering, ion beam sputtering, and evaporation. Studies include ion transport in thin-film electrolytes, electrodes, and electrode-electrolyte interfaces; electrical, dielectric, and optical properties of thin-film materials. Techniques include impedance spectroscopy, transient signal analysis, Raman scattering, infrared reflectance-absorption, optical spectroscopy, and scanning electron microscopy.

**183. SYNTHESIS AND PROPERTIES OF NOVEL CERAMIC AND NANOCOMPOSITE AND MACROMOLECULAR THIN FILMS**
J. B. Bates, N. J. Dudney, D. C. Lubben, F. A. Modine
(615) 574-6280 02-2 $495,000

Synthesis of thin films using combinations of physical vapor and chemical vapor deposition techniques such as ion beam sputtering and plasma polymerization. Types of films include (1) ceramic composites in which the phases are dispersed on a nanometer scale and (2) single-phase polymers composed of organic macromolecules combined with alkali-metal inorganic compounds in which the inorganic anion is incorporated into the polymer backbone. Films are characterized by a variety of optical, electrical, electron, and ion beam techniques including impedance spectroscopy, infrared reflectance-absorption spectroscopy, Raman scattering, scanning electron microscopy, and transmission electron microscopy.

**184. SYNTHESIS AND PROPERTIES OF NOVEL MATERIALS**
L. A. Boatner, M. M. Abraham, J. B. Brewster, B. C. Sales
(615) 574-5492 02-2 $1,155,000

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

**185. PHYSICAL PROPERTIES OF SUPERCONDUCTORS**
D. K. Christen, R. Feenstra, H. R. Kerchner, C. E. Klabunde, J. R. Thompson
(615) 574-6269 02-02 $460,000

Physical properties of superconductors, particularly high-$T_c$ materials, in various thin-film, single-crystal, melt-processed, magnetically aligned sintered, and composite forms. Configurations of thin films include epitaxial single-, multilayer, and superlattices. Irradiation of thin films and single crystals with energetic particles for the systematic introduction of flux pinning defect structures. Studies of flux pinning, magnetic relaxation, and critical currents are correlated with controlled defect arrays. Related investigations include fundamental superconducting properties such as upper and lower critical fields, magnetic penetration depths, and superconducting coherence length. Techniques and facilities include electrical transport by dc and pulsed current, with variable orientation of applied magnetic fields to 8T; dc magnetization using a SQUID-based instrument with 7-T capability; vibrating sample magnetometry to 9T; and ac susceptibility in superimposed dc fields to 5T.

**186. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION**
D. H. Lowndes, D. J. Eres, D. B. Geohegan, G. E. Jellison, D. P. Norton
(615) 574-6306 02-2 $960,000

Time-resolved ellipsometric measurements, light-assisted chemical vapor deposition of thin films, pulsed supersonic molecular beam deposition, modulated layered structures, superlattices, fabrication of superconducting and semiconducting thin films by laser ablation, laser-induced recrystallization of amorphous layers, thermal and laser annealing of lattice damage in semiconductors, fabrication of high-efficiency solar cells by laser, thick-film and thin-film techniques, effects of point defects and impurities on electrical and optical properties of single-crystal and polycrystalline Si, electrical, optical (including infra-red and luminescence spectroscopy), scanning tunneling microscopy, transmission electron microscopy, X-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering measurements, dopant concentration profiles, deep-level transient spectroscopy, and absolute quantum efficiency measurements.

**187. BULK SHIELDING REACTOR SHUTDOWN**
R. L. Stover, G. H. Coleman
(615) 574-8544 02-2 $474,000

This proposal is to provide funds for surveillance and shutdown of the BSR. Although the reactor core is defueled, there are 73 fuel assemblies stored in the reactor pool. Shutdown of the reactor requries removal of the fuel and other hazardous materials prior to transfer to the Surplus Facilities Management Program (SFMP). Until transfer occurs, surveliance is required in order to meet ES&H requirements and keep the facility and systems structurally sound.

**188. SMALL-ANGLE X-RAY SCATTERING**
G. D. Wignall, J. S. Lin, S. Spooner
(615) 574-5237 02-2 $210,000

Small-angle X-ray scattering of metals, metallic glasses, precipitates, alloys, ceramics, polymers, surfactants, fractal structures in polymers and oxide sols, domain structures in composites, dynamic deformation studies of polymers, time-slicing studies of phase transformation. Facilities are available to users at no charge for research published in the open literature or under contract for proprietary research.

**189. THEORY OF CONDENSED MATTER**
J. F. Cooke, H. L. Davis, T. Kaplan, S. H. Liu, G. D. Mahan, M. E. Mostoller, M. Rasolt, M. T. Robinson, R. F. Wood
(615) 574-5787 02-3 $989,000

Theory of nonequilibrium solidification in semiconductors, lattice vibrations in metals and alloys, lattice dynamics and potential energy calculations of ionic crystals, computer simulation of radiation damage, sputtering, and ion implanation surface studies with backscattered ions, development of LEED theory and interpretation of LEED data, surface vibrations and relaxation, electronic structure of metal surfaces, magnetism in transition metals and local moment systems, neutron scattering at high energies, electronic properties of mixed-valent and heavy fermion systems, high-temperature superconductivity, critical phenomena and phase transitions quantum Hall effect, diffusion and elastic vibrations of fractal systems, and self-organized critical systems. New directions include a study of the surface structure of disordered systems and the development of molecular dynamics theory and relevant computer programs for treating interfaces and, ultimately, crystal growth.

**190. STRUCTURAL PROPERTIES OF MATERIALS - X-RAY DIFFRACTION**
B. C. Larson, J. D. Budai, M. D. Galloway, J. Z. Tischler
(615) 574-5506 02-4 $278,000

Microstructure and properties of defects in solids, synchrotron X-ray scattering, time-resolved X-ray scattering, X-ray diffuse scattering, Mossbauer scattering spectroscopy, X-ray topography, neutron and ion irradiation induced defect clusters in metals, pulsed-laser-induced melting and crystal growth, defects associated with laser and thermal processing of pure and ion-implanted semiconductors, grain boundaries in semiconductors, microstructural characterization of high-temperature superconductors, anisotropic elastic theory of dislocation loops, calculation of diffuse scattering from dislocation loops and solute precipitates, energy-resolved X-ray scattering, quasi-elastic scattering, phase transformations, theory of scattering of X-rays from defects in solids.

**191. ELECTRON MICROSCOPY OF MATERIALS**
S. Pennycook, M. F. Chisholm, D. E. Jesson
(615) 574-5504 02-4 $864,000

Growth and relaxation phenomena in epitaxial thin films; interface structure/property relations in semiconductors and superconductors; morphological stability; molecular beam epitaxial growth; ion implantation; solid-hase recrystallization; segregation phenomena; electron energy loss spectroscopy; theory of elastic, inelastic and diffuse scattering of electrons from crystals and defects; Z-constrast image simulation.

**192. INVESTIGATIONS OF SUPERCONDUCTORS WITH HIGH CRITICAL TEMPERATURES**
D. K. Christen, L. A. Boatner, J. Brynestad, B. C. Chakoumakos, D. H. Lowndes, S. J. Pennycook, J. R. Thompson
(615) 574-6269 02-5 $605,000

Studies of superconducting materials with high transition temperatures. Synthesis, characterization, and anlysis of thin films, thin-film heterostructures, new substrate materials, single crystals and melt-processed bulk materials, and high-current conductors and composite structures. Magnetic and electrical transport properties, microstructural characterization by electron microscopy. Collaborative research with scientists at IBM Watson Research Center, General Electric Research, AT&T Bell Laboratories, American Superconductor Corporation, Intermagnetics General Corporation, the University of Tennessee, and other U.S. universities.

**193. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND RESEARCH CENTER**
D. B. Poker, T. P. Sjoreen, J. M. Williams, P. Withrow
(615) 576-8827 02-5 $1,799,000

The SMAC Collaborative Research Center provides facilities for materials alteration and characterization in a UHV environment. Methods which can be used for alteration include ion implantation and ion beam mixing using a multitude of ions and energies that span the range from 30 eV to ~5 MeV. 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.

**194. ION BEAM ANALYSIS AND ION IMPLANTATION**
C. W. White, T. E. Haynes, O. W. Holland, R. A. Zuhr
(615) 574-6295 02-5 $980,000

Studies of ion implantation damage and annealing in a variety of crystalline materials (semiconductors, metals, superconductors, insulators, etc.), formation of unique morphologies such as buried amorphous or insulating layers by high dose ion implantation, the use of high-energy ion beams to reduce the temperature of various thermally activated processes such as damage removal, alloying, and phase transformations; formation of buried compounds, studies of dose and dose rate dependence of damage accumulation during irradiation, characterization of superconducting thin films; fundamental studies of ion beam mixing in metal/semiconductor, metal/metal, and metal/insulator systems, applications of ion beam mixing and ion implantation to corrosion/catalysis studies, to reduction of friction and wear of metal surfaces, to changes in mechanical and optical properties of ceramics and insulators, and to reduction of corrosive wear of surgical alloys; studies of ion channeling phenomena; direct ion beam deposition (IBD) of isotopically pure thin films, epitaxial layers, and layered structures on metal and semiconductor substrates using decelerated, mass-analyzed ion beams; use of low-energy (10-200 eV) to alter surface atom mobilities and phase formation; studies of low-energy ion-solid interactions; formation of compound semiconductors, metallic layers, oxides, and nitrides by IBD.

**195. SURFACE PHYSICS AND CATALYSIS**
D. M. Zehner, A. F. Baddorf, H. L. Davis, J. F. Wendelken, J. K. Zuo
(615) 574-6291 02-5 $870,000

Studies of crystallographic and electronic structure of clean and adsorbate-covered metallic, intermetallic compounds, carbides, 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, lineshape analysis of Auger spectra, LEED, AES and X-ray photoelectron spectroscopy (XPS) studies of both clean and adsorbate-covered surfaces, determination of effects of intrinsic and extrinsic surface defects on surface properties and surface and thin-film growth morphology using high-resolution LEED, vibronic structure of surfaces and adsorbates examined by high-resolution electron energy loss spectroscopy (EELS), examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

**Materials Chemistry - 03 -**

M. L. Poutsma - (615) 574-5028

**196. CHEMISTRY OF ADVANCED INORGANIC MATERIALS**
E. J. Kelly, C. E. Bamberger, J. Brynestad, L. Maya, C. E. Vallet
(615) 574-5024 03-1 $1,083,000

Systematic studies of electrocatalysts for various reactions of interest in energy conversation/storage, environmental clean-up, and energy intensive chemical production industries; generation of new electrocatalysts by ion implantation/ion beam mixing techniques and their characterization by Rutherford backscattering and XPS/Auger spectroscopies; in situ real-time analysis of the electroctalytic processes (reaction kinetics and mechanism, electrocatalytic activity, electronic and structural properties) by electrochemical techniques, photoacoustic/photothermal-deflection spectroscopies, and scanning tunneling microscopy. Synthesis of whiskers and platelets for direct use as reinforcing agents in composite materials or as precursors in morphostatic conversions, i.e., reactions in which the product retains the morphology of the precursor; CrN and $Cr_3C_2$ platelets have been obtained from $Cr_3C_2$, and whiskers of sodium tungsten bronzes are under study as precursors to tungsten carbide whiskers. Development of new generalized methodologies for the synthesis of nonoxidic ceramic and electronic materials with particular emphasis on plasma processing for chemical vapor deposition of films (e.g., SiC or cubic BN). Synthesis and characterization of high-$T_c$ superconductors; composition/kinetics/phase formation/property relationships and their significance in the attainment of high current densities in high magnetic fields.

**197. NUCLEATION, GROWTH, AND TRANSPORT PHENOMENA IN HOMOGENEOUS PRECIPITATION**
C. H. Byers, O. A. Basaran, M. T. Harris
(615) 574-4653 03-2 $292,000

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

**198. THERMODYNAMICS AND KINETICS OF ENERGY-RELATED MATERIALS**
T. B. Lindemer
(615) 574-6850    03-2 $311,000

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

**199. STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS**
A. H. Narten, B. K. Annis, A. Habenschuss, D. W. Noid, B. G. Sumpter, B. Wunderlich
(615) 574-4974    03-2 $1,177,000

Characterization of polymers and composites at the molecular level by neutron and X-ray scattering, thermal analysis, atomic force microscopy, and statistical mechanical calculations. Structural relationships between crystalline, partially ordered, and amorphous regions. Simulation of polymer chain dynamics in large-scale molecular dynamics calculations. Improvement of the basic understanding of local molecular structure, the packing of chains in semicrystalline polymers, and the dynamics of materials ranging from oriented fibers to isotropic materials. Materials studied include high-performance crystalline fibers and composites, liquid crystalline, and plastic crystalline mesophases. Development of methods of predicting polymer properties resulting from various processing methods.

**200. BLENDS OF MACROMOLECULES WITH NANOPHASE SEPARATION**
A. H. Narten, J. G. Curro, K. S. Schweizer
(615) 574-4974    03-2 $250,000

Development of a scientific basis for the molecular design of polymer blends in order to optimize physical and end-use properties. Prediction of molten blend structure, miscibility, phase diagrams and other thermodynamic properties from integral equation theories. Testing of theoretical predictions by neutron and X-ray scattering. Focus on multicomponent polymer systems where mixing occurs on molecular length scales in contrast to conventional composites and filled polymers.

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**Facility - 04 -**

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**201. ADVANCED NEUTRON SOURCE**
C. D. West, M. L. Gildner, R. M. Harrington, J. B. Hayter, B. H. Montgomery, D. L. Selby, P. B. Thompson
(615) 574-0370    04-1 $24,255,000

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

## PACIFIC NORTHWEST LABORATORY

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**Metallurgy and Ceramics - 01 -**

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**202. MICROSTRUCTURAL MODIFICATION IN CERAMIC PROCESSING USING INORGANIC POLYMER DISPERSANTS**
G. J. Exarhos, I. A. Aksay (Princeton Univ.), W. D. Samuels
(509) 375-2440    01-1 $412,000

Fundamental studies of particle compaction phenomena in colloidal dispersions and synthesis of inorganic polymer ceramic molecular composites. Localized particle-polymer solvent interactions probed by means of in situ molecular spectroscopic measurements. Integration of spectroscopic data with particle compaction measurements is used to evaluate packing efficiency and relate it to chemical functionality of derivatized inorganic polymer dispersants. Behavior of bound polymers in the greenbody to high temperatures during sintering is a principal research area. Improvement in mechanical properties of the fired ceramic is correlated with void density and distribution which evolves during processing and with the generation of interfacial phases formed by incorporation of the inorganic polymer with the ceramic matrix.

**203. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS**
R. H. Jones, D. R. Baer, C. H. Henager Jr., E. P. Simonen, C. F. Windisch
(509) 376-4276    01-2 $445,000

Investigations of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium nickel, nickel-based alloys, and ceramic matrix composites in gaseous and aqueous environments. Relationships between interfacial and grain boundary chemistry, hydrogen embrittlement, and intergranular stress corrosion cracking investigated with surface analytical tools, electrochemical polarization, straining electrode tests, subcritical crack growth tests, and crack-tip and fracture surface analysis. Modeling of the electrochemical conditions at the tip of a growing crack and evaluation of the electrochemical behavior of sulfur and phosphorus in the grain boundaries of nickel and iron. Acoustic emission and differential, reversed dc potential drop analysis of stress corrosion initiation and cracking processes. Effect of surface chemistry on gas phase adsorption and aqueous corrosion using in situ AES/XPS and corrosion side-cell.

**204. CHEMISTRY AND PHYSICS OF CERAMIC SURFACES**
L. R. Pederson, B. C. Bunker, K. F. Ferris
(509) 375-2731    01-3 $392,000

Study of the chemistry and physics of specific crystalline oxide bonding configurations with an emphasis on the properties of defects. Colloid chemistry, surface science, and theoretical methods are coupled to generate a comprehensive understanding of oxide surface chemistry. Model surfaces of metal oxides are created by cleavage of single crystals. Hydration/solvation, ion adsorption, acid/base chemistry, and site stabilities/reconstruction of these model surfaces are investigated. Surfaces are characterized using electron and vibrational spectroscopies; electron diffraction; scanning tunneling microscopy; electron, photon, and thermal desorption methods; and microcalorimetry. Molecular modeling activities emphasize ab initio electronic structure and molecular dynamics approaches, and include the development of methodologies for large-scale assemblies.

**205. IRRADIATION-ASSISTED STRESS CORROSION CRACKING**
S. M. Bruemmer, J. L. Brimhall, E. P. Simonen
(509) 376-0636    01-4 $485,000

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

**206. IRRADIATION EFFECTS IN CERAMICS**
W. J. Weber, N. J. Hess
(509) 375-2299    01-4 $150,000

Multidisciplinary research on the production, nature, and accumulation of irradiation-induced defects, microstructures, and solid-state transformations in ceramics. Irradiations with neutrons, ions, and electrons to study point defect production and associated effects from both single displacement events and high-energy displacement cascades. Develop understanding of structural stability and irradiation-induced amorphization in ceramics. Computer simulations of defect production/survivability, defect stability, and defect migration. The investigations utilize X-ray and neutron diffraction, electron microscopy, EXAFS, laser spectroscopies, ion-beam techniques, and electrical property measurements to characterize the defects, microstructures, and transformations introduced by irradiation in simple and complex oxides, carbides, and nitrides. Work includes the development of techniques for in situ characterization during neutron and ion-beam irradiations.

**Solid State Physics - 02 -**

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

**207. THIN FILM OPTICAL MATERIALS**
G. J. Exarhos, K. F. Ferris, N. J. Hess
(509) 375-2440 02-2 $247,000

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

**Materials Chemistry - 03 -**

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

**208. CERAMIC COMPOSITE SYNTHESIS UTILIZING BIOLOGICAL PROCESSES**
P. C. Rieke, A. I. Caplan, A. I. Caplan,
A. H. Heuer (Case Western), B. J. Tarasevich (PNL)
(509) 375-2833 03-1 $647,000

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

## SANDIA NATIONAL LABORATORIES-ALBUQUERQUE

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**Metallurgy and Ceramics - 01 -**

G. A. Samara - (505) 844-6653

**209. ATOMIC LEVEL SCIENCE OF INTERFACIAL ADHESION**
T. A. Michalske, B. W. Dodson, J. E. Houston,
J. Nelson, N. D. Shinn, R. C. Thomas
(505) 844-5829 01-2 $500,000

The goal of this program is to understand, in atomic detail, the nature of the physical and chemical interactions that bind solid surfaces together. This study includes atomic scale measurements of interfacial bonding forces, theoretical calculations of interfacial bonding, surface science measurements of interfacial bonding and structure, and macroscopic adhesion measurements that will be used to relate the results of fundamental theory and experiment to more conventional measures of adhesion. Key to our approach is the ability to make detailed measurements of interfacial force profiles on well controlled and characterized interfaces. These measurements provide a common point for investigations ranging from first principles theory to practical adhesion and provide fundamental insight into the factors controlling interfacial adhesion..

**210. PHYSICS AND CHEMISTRY OF CERAMICS**
D. W. Schaefer, T. L. Aselage, R. A. Assink,
C. J. Brinker, A. J. Hurd, M. L. F. Phillips,
P. R. Schunk, R. W. Schwartz
(505) 844-7937 01-2 $1,259,000

Multidisciplinary studies to relate molecular structure of ceramics to physical properties. One objective is to develop a fundamental understanding of the precursor preparation and consolidation processes required to produce novel and superior ceramics. Both solution and gas-phase processes are studied. A second objective is to use fundamental understanding of processing to prepare new and improved ceramics such as high temperature superconductors. Characterize sol-to-gel and gel-to-glass transitions in the silica system using SAXS, NMR, and light scattering to determine structures of the pre-gel phase, random colloidal aggregates, and the gel-to-glass conversion; model structure of porous materials using concepts of fractal geometry to predict structure from solution chemistry, and model sintering and absorption characteristics of random porous materials. Study formation of fine-particle ceramics by aeorsol techniques. Prepare ceramic superconductors and other electronic ceramics by novel solution processing. Study phase relationships and interfacial reactions in ceramic superconductors and other electronic ceramics.

**211. ENERGETIC-PARTICLE SYNTHESIS AND SCIENCE OF MATERIALS**
S. M. Myers, J. C. Barbour, R. J. Bourcier, B. L. Doyle, M. T. Dugger, D. M. Follstaedt, J. A. Knapp, D. A. Redman, H. J. Stein, W. R. Wampler
(505) 844-6076 01-3 $953,000

Basic research is conducted on the interactions of ion, laser, electron, and plasma beams with metals, semiconductors and dielectrics. The synthesis of new or novel metastable and equilibrium microstructures in solids with energetic ions, remote plasma sources and pulsed laser deposition is studied. Both the evolution and final states of these systems are characterized by ion-beam analysis, TEM, EPR, optical absorption, X-ray scattering, AES, XPS, time-resolved reflectivity, time-resolved electrical conductivity, and mechanical and electrochemical testing. These methods are utilized for fundamental studies of metastable amorphous and crystalline alloys, superlattices, defects in semiconductors, synthesis of novel layered structures, rapid-solidification processes in semiconductors and metals, properties of hydrogen in materials, and mechanical and chemical effects. Predictions of consequences are developed for semiconductor devices and sensors, fusion energy, hydrogen storage, coatings technology and corrosion.

**212. ADVANCED GROWTH TECHNIQUES FOR IMPROVED SEMICONDUCTOR STRUCTURES**
S. T. Picraux, D. K. Brice, S. A. Chalmers, E. Chason, B. W. Dodson, B. Swartzentruber, J. Y. Tsao
(505) 844-7681 01-3 $355,000

Advanced growth techniques are studied for the synthesis of new and improved epitaxial semiconductor heterostructurs. In situ diagnostics and new growth techniques are used in conjunction with molecular beam epitaxy (MBE) to grow new semiconductor structures. By combining energetic beams with MBE, new approaches to controlling the growth process as well as new understanding of the defect-mediated mechanisms controlling growth are developed. Studies concentrate on Ge and Si, as well as layered III-V compounds and SiGe strained layer structures. A primary purpose of this research is to provide new understanding of fundamental epitaxial growth mechanisms and new methods and diagnostics for the growth of improved epitaxial layered structures. Advanced in situ techniques yield surface structure, composition and chemical reactivity information and corrleation with growth parameters. Theoretical studies model the growth processes and address growth mechanisms in order to interpret and guide the experimental studies.

**213. STRAINED-LAYER SEMICONDUCTOR MATERIALS SCIENCE**
P. L. Gourley, I. J. Fritz, E. D. Jones, S. K. Lyo, J. S. Nelson, R. Schneider
(505) 844-4309 01-5 $404,000

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

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**Solid State Physics - 02 -**

G. A. Samara - (505) 844-6653

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**214. PHYSICS AND CHEMISTRY OF NOVEL SUPERCONDUCTORS**
D. S. Ginley, J. S. Martens, B. Morison, J. E. Schirber, E. B. Stechel, C. P. Tigges, E. L. Venturini
(505) 844-6653 02-2 $618,000

The fundamental physical properties of the oxide-based high temperature superconductors with emphasis on the thallium system. Directed toward understanding the detailed electronic band structure, doping flux motion and pinning, and carrier transport in these materials, especially as they pertain to understanding metal-insulator transitions, superconductivity, and the role of oxygen in determining transport properties. Some effort is also devoted to organic superconductors. Unique and specialized instrumental capabilities including conductivity, magnetization, ESR, magnetotransport, de Haas van Alphen, thermopower and tunneling. Experiments at temperatures as low as 0.05 K, magnetic fields up to 120 kOe and hydrostatic pressure to 10 kbar in various combinations. An active in-house synthesis program; unique processing capabilities including high pressure, high temperature oxygen.

**215. TAILORED SURFACES AND INTERFACES FOR MATERIALS APPLICATIONS**
T. A. Michalske, P. J. Feibelman, J. E. Houston, G. L. Kellogg, T. M. Mager, N. D. Shinn, B. Swartzentruber
(505) 844-5829 02-2 $633,000

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

**216. BORON-RICH SOLIDS**
D. Emin, T. L. Aselage, B. Morosin, G. A. Samara, A. C. Switendick, D. R. Tallant, H. L. Tardy, E. L. Venturini
(505) 844-6653 02-5 $516,000

This program investigates boron-rich solids which are refractory materials with uncoventional bondings, structures and properties. The goal is to understand these novel materials and assess their potential for applications. The investigations primarily focus on semiconducting boron carbides, insulating borides including the wide-gap icosahedral boron pnictides, and other refractory borides, such as diborides and hexaborides. The materials are synthesized by a variety of techniques. The structural properties, electronic structure, electronic transport (conductivity, Hall effect and seebeck coefficient measurements) dielectric, optical, magnetic and ultrasonic properties, thermal conductivity and specific heat will be investigated.

**Materials Chemistry - 03 -**

J. B. Gerardo - (505) 844-3871

**217. CHEMICAL VAPOR DEPOSITION SCIENCES**
M. E. Bartram, W. G. Breiland, M. E. Coltrin, J. R. Creighton, G. H. Evans, P. Ho, R. J. Kee, K. P. Killeen, J. E. Parmeter
(505) 844-5857 03-3 $812,000

Studies of important vapor-phase and surface reactions during CVD deposition under conditions used to fabricate photovoltaic cells, wear- and corrosion-resistant coatings, and semiconductor devices. Measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Development of predictive numerical models, which include chemical kinetics and fluid dynamics. Application of a wide array of laser-based measurement capabilities to the study of vapor phase and surface reactions of these processing techniques and application of surface measurement techniques to study the product materials.

## SANDIA NATIONAL LABORATORIES-LIVERMORE

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**Metallurgy and Ceramics - 01 -**

**218. SURFACE, INTERFACE, AND BULK PROPERTIES OF ADVANCED CERAMICS**
R. H. Stulen, J. C. Hamilton, K. F. McCarty
(510) 294-2070 01-1 $191,000

The goal of this task is two fold: (1) to develop a more complete understanding of the surface, interface, and bulk properties of advanced ceramics, and (2) to synthesize novel, thin-film ceramic structures. Current emphasis is placed on two important material systems:
(1) high-temperature superconductors and
(2) ultrahard ceramics. The diagnostic techniques utilized are primarily optical and include Raman spectroscopy and infrared spectroscopy for the study of phase composition and structure. Detailed temperature measurements of the phonon scattering and electronic scattering of ceramic and fullerene superconductors provide fundamental characterization of the lattice effects (extent of electron-phonon coupling and anharmonicity) and superconducting properties (magnitude of energy gap). The second portion of this program examines

the formation and properties of thin films synthesized by the emerging technique of pulsed laser deposition. Current emphasis is on the formation of phase-pure films of the metastable phase cubic boron nitride. Superlattices of ceramic materials will also be synthesized and characterized. In situ diagnostics in the growth chamber (low energy electron diffraction, Auger spectroscopy, and infrared spectroscopy) are used to determine the relationship between the deposition parameters (rate, temperature, energy of depositing species, etc.) and the film properties (phase, elemental composition, degree of epitaxy, etc.)

**219. DEFECTS AND IMPURITIEIS IN SOLIDS/COMPUTATIONAL MATERIALS SCIENCE/VISTING SCIENTIST PROGRAM**

W. G. Wolfer, S. Baller, D. C. Chrzan, M. S. Daw, T. E. Felter, S. M. Folles, R. Q. Hwang, M. J. Mills, C. M. Rohlfing, A. F. Wright
(510) 294-2307 01-2 $1,215,000

Unique experimental and theoretical tools developed in this program are combined to study structural defects and impurities in solids and on surfaces. The experimental tools are high-resolution transmission electron microscopy (HRTEM), high and medium energy ion scattering facilities, video low-energy electron diffraction (LEED) with I-V capability, surface analytical tools, scanning tunneling microscopy (STM), and low energy electron microscopy (LEEM). Theoretical tools developed and employed include quantum chemistry codes, LDA/pseudo-potential methods, the embedded atom method (EAM), and the cluster functional (CFM) methods for large-scale atomistic computer simulations. These experimental and theoretical capabilities are utilized to study grain boundaries, interfaces and surfaces in metal alloys and intermetallic compounds, impurity segregation to these boundaries, and the interactions with dislocation, gas bubbles and defect clusters. Growth of metal layers on substrates are investegated using STM, LEED, and LEEM and theoretical models are developed for the nucleation and growth of kinetics of thin film layers. HTREM, in conjunction with large scale computer simulations, are performed to resolve the dislocation core structure in intermetallic compounds and to analyze the dislocation network configurations and evolution during plastic deformation. Many of the results generated by this research program are utilized in concurrent development and engineering projects at Sandia or other national laboratories. In addition, the dissemination to materials science programs at universities to industrial research and development laboratories is conducted through the Visting Scientist Program.

**220. ALLOY THEORY**

D. D. Johnson, J. D. Althoff, F. J. Pinski (Univ. of Cincinnati)
(510) 294-2751 01-3 $390,000

A "first-principle" theory for alloys is developed in which charge transfer and magnetic interactions between the alloy constituents play an essential role in determining the phase diagrams and the ordering tendencies. Correlation functions for compositional and magnetic ordering are derived from the theory and utilized to interpret experimental magnetic ordering are derived from the theory and utilized to interpret experimental results from diffuse X-ray and neutron scattering experiments and to further plan and guide such experiments. The combined theoretical and experimental efforts elucidate the underlying electronic forces for intermetallic interactions and their influence on the thermodynamics of alloys. Finally, the theory will be used to explore and discover new metal alloys.

**Solid State Physics - 02 -**

**221. ADVANCED OPTICAL DIAGNOSTICS FOR INTERFACES AND THIN FILMS**

R. H. Stulen, R. J. Anderson, J. C. Hamilton
(510) 294-2070 02-2 $241,000

Develop, evaluate, and apply advanced, nonperturbing diagnostic techniques for studying the structure and dynamics of advanced materials. The scope includes studies of bulk, interface, and surface properties using spectroscopic techniques. We emphasize the use of these techniques to characterize electronic structure, ultrafast dynamics, and the chemistry of surfaces and interfaces formed during thin film growth. The approach includes the use of 1) ultrashort laser pulses, extending to the femtosecond regime, to examine excited state dynamics, 2) infrared absorption and emission to probe molecular vibrations at surfaces and interfaces, and 3) impulsively stimulated scattering to study mechanical properties and thermal conductivity of thin films. Materials under investigation include semiconductors, nonlinear optical materials, and large bandgap systems, and their interfaces with metals.

## STANFORD SYNCHROTRON RADIATION LABORATORY

**Stanford University**
**Stanford, CA 94309-0210**

A. I. Bienenstock - (415) 926-3153
Fax No.: (415) 926-4100

**Facility Operations - 04 -**

**222. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES**
A. I. Bienenstock, H. Winick
(415) 926-3153 04-1 $3,144,000

Support of materials research utilizing synchrotron radiation, as well as operations and development of the Stanford Synchrotron Radiation Laboratory (SSRL). Development and utilization of new methods for determining atomic arrangement in amorphous materials, and on surfaces, time-resolved studies of thin film growth, 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. Performance and photoelectron spectroscopic studies of catalysts. Development and improvement of accelerators and insertion devices for synchrotron radiation production, and development and Lau diffraction for time-resolved protein crystallography. Development of ultra-high resolution scattering techniques, by means of resonant nuclear scattering.

# SECTION B

Grant Research

(Primarily Universities)

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

## ALFRED UNIVERSITY
**Alfred, NY 14802**

**223. STRUCTURE, STOICHIOMETRY AND STABILITY IN MAGNETOPLUMBITE AND B-ALUMINA TYPE CERAMICS**
A. N. Cormack, Department of Ceramic Science and Engineering
(607) 871-2180 01-1 $90,157

Atomistic simulation of defect structures and energies for defect clusters in mirror planes of magnetoplumbite and β-alumina structures; defect cluster interaction. Born model with shell model treatment of atomic polarizations; atomic relaxation treated by Mott-Littleton approximation. Barium, strontium and calcium hexa-aluminates ($MAl_{12}O_{19}$) calculated.

## ARIZONA STATE UNIVERSITY
**Tempe, AZ 85287**

**224. SOLID ELECTROLYTES AND IMPACT-RESISTANT CERAMICS**
C. A. Angell, Department of Chemistry
(602) 965-7217 01-1 $89,848

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

**225. HIGH RESOLUTION ENERGY LOSS RESEARCH: SI COMPOUND CERAMICS AND COMPOSITES**
R. W. Carpenter, Center for Solid State Science
(602) 965-4546

S. H. Lin, Department of Chemistry
(602) 965-3715 01-1 $95,568

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

**226. SURFACE STRUCTURES AND REACTIONS OF CERAMICS AND METALS**
J. M. Cowley, Department of Physics
(602) 965-6459 02-2 $50,000

Studies of surface structures of oxides and metals and solid-solid interfaces using a range of advanced electron-optical techniques, including: conventional scanning and transmission microscopy, scanning reflection electron microscopy, reflection electron energy loss spectroscopy, nanodiffraction and shadow imaging and analysis and off-line electron holography.

## UNIVERSITY OF ARIZONA
**Tucson, AZ 85721**

**227. ARTIFICIALLY STRUCTURED MAGNETIC MATERIALS**
C. M. Falco, Department of Physics
(602) 621-6771 02-2 $90,000

Emphasis on understanding magnetism using well characterized surfaces and interfaces and in developing artificially structured magnetic materials with improved properties. Preparation of artificially structured magnetic materials: Molecular Beam Epitaxy (MBE); multi-target sputtering. Sample characterization: various X-ray diffraction techniques, Scanning Tunneling Microscopy, Auger, X-ray Photoelectron Spectroscopy, Ion Scattering Spectroscopy, and Secondary Ion Mass Spectroscopy, Reflected High and Low Energy Electron Diffraction, Rutherford Backscattering, Scanning and Electron Transmission Microscopy. Magnetic properties of ultra-thin magnetic films and surfaces; interfaces in multilayers and superlattices using in situ Surface Magneto-Optic Kerr Effect, variable-temperature Vibrating Sample Magnetometry, Brillouin Light Scattering, Magnetic Neutron Scattering and Synchrotron Photoemission.

## BOEING COMPANY
**M.S.2-T-05, P.O. Box 3999**
**Seattle, WA 98124**

**228. X-RAY SPECTROSCOPIC INVESTIGATION OF AMORPHIZED MATERIALS**
R. B. Greegor, Department of Physics
(206) 544-5307

F. W. Lytle, Department of Physics
(206) 544-5348 01-1 $60,885

EXAFS/XANES techniques are used to determine the structural arrangements in synthetically produced materials, including ion-implanted materials having phases similar to naturally occurring metamict minerals (e.g., titanite, pyrochlore, zircon). Investigation of Pb implanted crystalline Pb pyrophosphate and glassy Pb pyrophosphate. Metal-metal bonding examined in proton irradiated Ni and Ti aluminides. Site speciation examined in radwaste forms, including doped perovskite, synroc and in-situ virtrified glass. Development of optical EXAFS for differentiation of an atom on damaged and undamaged sites.

## BOSTON UNIVERSITY
**500 Commonwealth Avenue**
**Boston, MA 02215**

**229. THE HEAVY ELECTRON STATE**
A. Auerbach, Department of Physics
(617) 353-5787 02-3 $38,119

Heavy electron compounds will be investigated, particularly the transition to the Fermi-liquid state. The role of intersite magnetic interactions and the Fermi-liquid state will be investigated by using a time dependent functional integral methodology.

**230. INVESTIGATION OF THE STRUCTURE AND DYNAMICAL TRENDS IN THE GROWTH OF TRANSITION METAL OVERLAYERS AND SURFACE MAGNETIC STRUCTURE OF INSULATORS BY HE BEAM SCATTERING SPECTROSCOPIES**
M. M. El-Batanouny, Department of Physics
(617) 353-4721 02-4 $97,800

Use of scattered spin-polarized metastable He($2^3S$) atoms from surfaces both elastically and inelastically, to study the structural, dynamic and magnetic trends of the 3-d transition metal overlayers-Cu, Au, Ag and Cr on Pd(111) and Pd(110) substrates; and Pd and Cu on a Nb(110) substrate. Magnetic properties will be studied in the newly constructed Spin-Polarized Metastable He (SMPH) facility. The surface magnetic structure of antiferromagnetic transition metal oxides (example, MnO) will be studied. Computer modeling, employing Friedel oscillations and Double-sine-Gordon surface dislocations, will be used to interpretate measured phonon dispersion data.

## BROWN UNIVERSITY
**Providence, RI 02912**

**231. HIGH TEMPERATURE FATIGUE CRACK GROWTH IN CERAMICS AND CERAMIC-MATRIX COMPOSITES**
S. Suresh, Division of Engineering
(401) 863-2626 01-2 $113,405

Experimental and theoretical investigation of stable crack growth under static and cyclic tensile loads in monolithic and ceramic matrix composites up to 1500 C. Effects of loading rate/cyclic frequency, hold time, cyclic means stress and test temperature on rates of subcritical crack growth; characterization of crack advance by fracture mechanics; characterization of crack-tip damage by transmission electron microscopy; effects of pre-existing amorphous films and amorphous films formed at test temperature. Finite element simulations of evolution of cyclic damage zones ahead of tensile fatigue cracks using constitutive formulations to represent experimentally determined damage mechanisms.

**232. SURFACES AND THIN FILMS STUDIED BY PICOSECOND ULTRASONICS**
H. J. Maris, Department of Physics
(401) 863-2185

J. Tauc, Department of Physics
(401) 863-2318 02-2 $144,000

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

## UNIVERSITY OF CALIFORNIA AT DAVIS
**Davis, CA 95616**

**233. INVESTIGATION OF THE RATE-CONTROLLING MECHANISM(S) FOR HIGH TEMPERATURE CREEP AND THE RELATIONSHIP BETWEEN CREEP AND MELTING BY USE OF HIGH PRESSURE AS A VARIABLE**
H. W. Green, Department of Geology
(916) 752-1863

A. K. Mukherjee, Department of Mechanical Engineering
(916) 752-1776 01-2 $112,640

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

**234. INVESTIGATION OF RADIATION DAMAGE AND DECOMPOSITION OF CERAMICS USING ELECTRON MICROSCOPY**
D. G. Howitt, Department of Mechanical Engineering
(916) 752-1164 01-4 $83,599

Investigation of electron induced radiolysis, ionization, displacement damage, diffusion and stimulated desorbtion by means of in-situ analytical electron microscopy and mass spectroscopy. Study of scribing at high beam current density. Materials include dielectrics and semiconductors. Study of free standing ceramics thin films.

## UNIVERSITY OF CALIFORNIA AT IRVINE
**Irvine, CA 92717**

**235. MECHANISMS OF HIGH TEMPERATURE RUPTURE UNDER MULTIAXIAL STRESS**
J. C. Earthman, Department of Mechanical Engineering
(714) 856-5018

F. A. Mohamed, Department of Mechanical Engineering
(714) 856-5807 01-2 $81,000

Mechanisms of high temperature rupture and damage under different multiaxial stress states in Ni, 304 SS and $Ni_3Al$. Examination of cavity density, cavity distribution, cavitating grain boundary facet size and orientation, and rupture surface topography for three states of stress. Correlation of stress state with time to rupture. Grain boundary sliding mechanisms. Evaluation of effect of multiaxial stresses on the role of intergranular particles. Analysis of the role of cavity nucleation.

**236. OPTICAL STUDIES OF MOLECULAR ADSORBATES**
J. C. Hemminger, Department of Chemistry
(714) 856-6020 02-2 $70,000 (7 months)

Optical probes including Raman scattering spectroscopy and laser induced thermal desorption with Fourier transform mass spectrometry detection, scanning tunneling microscopy and conventional methods of UHV surface science will be combined to study molecular adsorbates on well characterized metal surfaces and in ultrathin films to identify the fundamentals necessary to allow the controlled preparation of anisotropic ultrathin films of organic monomers. The effect of substrate atomic structure on the ordering of the adsorbates will be determined. Of particular interest is the effect of substrate defects on the orientational ordering of adsorbates.

**237. INELASTIC ELECTRON SCATTERING FROM SURFACES**
D. L. Mills, Department of Physics
(714) 856-5148 02-3 $114,000

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 Mills and Professor Tong at the University of Wisconsin at Milwaukee.

## UNIVERSITY OF CALIFORNIA AT LOS ANGELES
**5732 Boelter Hall**
**Los Angeles, CA 90025**

**238. MECHANICAL BEHAVIOR OF ION-IRRADIATED ORDERED INTERMETALLIC COMPOUNDS**
A. J. Ardell, Department of Materials Science and Engineering
(213) 825-7011 01-4 $99,447

Correlation between mechanical behavior and microstructure of ion irradiated intermetallic compounds. Specimens tested by miniaturized disk-bend test (MDBT) apparatus. Hardness and modulus measured as functions of irradiation dose.

Effect of irradiation-induced disordering on grain boundary cohesive strength and cleavage. Development of a miniaturized disk-bend fatigue apparatus.

**239. APPLICATIONS OF MESOSCOPIC PHYSICS TO NOVEL CORRELATIONS AND FLUCTUATION OF SPECKLE PATTERNS: IMAGING AND TOMOGRAPHY WITH MULTIPLY SCATTERED CLASSICAL WAVES**
SheChao Feng, Department of Physics
(213) 825-8530 02-3 $57,000

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

## UNIVERSITY OF CALIFORNIA AT SAN DIEGO
**La Jolla, CA 92093-0319**

**240. PREPARATION AND CHARACTERIZATION OF SUPERLATTICES**
I. K. Schuller, Department of Physics
(619) 534-2540 02-2 $110,000 (3 months)

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

**241. ION MIXING OF SEMICONDUCTOR LAYERED-STRUCTURES**
S. S. Lau, Department of Electrical Engineering and Computer Sciences
(619) 534-3097 02-4 $75,000 (9 months)

Experimental investigation of layer disordering by ion mixing in semiconductor quantum-well and superlattice structures. Emphasis is on determining the disordering mechanisms of semiconductor layered-structures under ion bombardment. Issues being addressed include the interplay between defects under thermal equilibrium and those generated by ion mixing and exploitation of thermally activated ion mixing to effect layer mixing in quantum-wells and superlattices. A goal is to develop a unified mechanism for ion mixing in such materials.

## UNIVERSITY OF CALIFORNIA AT SANTA BARBARA
**Santa Barbara, CA 93106**

**242. FUNDAMENTAL STUDIES OF THE INTERRELATIONSHIP BETWEEN GRAIN BOUNDARY PROPERTIES AND THE MACROSCOPIC PROPERTIES OF POLYCRYSTALLINE MATERIALS**
D. R. Clarke, Materials Department
(805) 893-8232 01-1 $113,000

Relationships between properties of individual grain boundaries and macroscopic properties of polyphase, polycrystalline materials. Measurement of electrical properties and plastic deformation of grain boundaires in bicrystals as a function of bicyrstallography determined by electron channeling and high resolution transmission electron microscopy. Results will be compared to those obtained from polycrystalline thin films and compared to simulation results.

**243. RESEARCH IN THEORIES OF PATTERN FORMATION AND NONEQUILIBRIUM PHENOMENA**
J. S. Langer, Department of Physics
(805) 893-2280 02-3 $108,000

Theoretical investigations of phenomena that occur in systems far from thermodynamic or mechanical equilibrium. Dendritic solidification with emphasis on the prediction of microstructural pattern formation in alloys. Statistical theories of nonequilibrium phenomena in complex systems. Dynamics of systems driven persistently toward the threshold of instability.

**244. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS**
D. J. Scalapino, Department of Physics
(805) 893-2871

R. L. Sugar, Department of Physics
(805) 893-3469 02-3 $73,500 (9 months)

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

**245. MOLECULAR PROPERTIES OF THIN ORGANIC INTERFACIAL FILMS**
J. Israelachvili, Department of Chemical and Nuclear Engineering
(805) 961-3412 03-1 $153,000

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

**246. INTERFACIAL PROPERTIES OF CHARGED MACROMOLECULES**
P. A. Pincus, College of Engineering-Engineering Materials Program
(805) 893-4685 03-2 $83,000

Theoretical research on the interaction of polymers with surfaces. Effects of long rearrangement times leading to quasi=irreversibility and hysteresis in the force between polymer clad surfaces. Polymer adsorbed on fluid-fluid interfaces. Dispersion stability of suspended colloids with adsorbed polymers. Interaction of charged polymers with surfaces, where Coulombic forces are central to the interactions which control the physical behavior.

## UNIVERSITY OF CALIFORNIA AT SANTA CRUZ
**Santa Cruz, CA 95064**

**247. PHASE TRANSITIONS IN SYSTEMS WITH QUENCHED DISORDER**
D. Belanger, Department of Physics
(408) 459-2871 02-1 $68,000

Investigation of phase transitions in the presence of quenched defects in well controlled and characterized systems using neutron scattering, optical birefringence, optical Faraday rotation, capacitance and pulsed specific heat. Systems include crystals where antiferromagnetism and spin-glass behavior are in coexistence, epitaxial antiferromagnetic thin films, magnetic dipolar materials, and stacked trangular lattice antiferromagnets.

## CALIFORNIA INSTITUTE OF TECHNOLOGY
**Pasadena, CA 91125**

**248. ORDERING PHENOMENA IN UNDERCOOLED ALLOYS**
B. T. Fultz, Engineering Department
(818) 356-2170 01-1 $73,752

Study of kinetics of disorder -> order transformations in rapidly quenched alloys. Alloys studied include $Fe_3Al$, $Fe_3Si$, and $Ni_3Al$. Measurement of long-range order (LRO) by X-ray diffractometry, and short-range order (SRO) by $_{57}Fe$ Mossbauer spectrometry and extended electron energy loss fine structure (EXELFS) spectrometry. Kinetic path of ordering obtained through the two-dimensional space spanned by the SRO and LRO parameters. Measurement of difference in vibrational entropy of disordered and ordered alloys by low temperature calorimetry and temperature-dependent EXELFS spectrometry.

**249. STUDIES OF ALLOY STRUCTURES AND PROPERTIES**
W. L. Johnson, Division of Engineering and Applied Science
(818) 356-4433 01-1 $201,740

Synthesis, characterization, and properties of metastable metallic materials. Amorphous and nanocrystalline materials studied. Solid state amorphization by interdiffusion reactions, hydriding, and mechanical alloying and attrition. Physical properties. Wear-induced amorphization and effect of surface structure on sliding friction. Consolidation of amorphous alloy powders produced by mechanical alloying and mechanical attrition. Mechanical testing, computer modeling, and molecular dynamics. Techniques include electron microscopy, X-ray diffraction, small angle X-ray diffraction, and neutron and electron diffraction.

**250. IRRADIATION - INDUCED TRANSFORMATIONS IN THIN FILMS**
H. A. Atwater, Department of Applied Physics
(818) 356-2197 01-4 $105,430

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

**251. MELTING IN ADSORBED FILMS**
D. L. Goodstein, Department of Physics, Mathematics, and Astronomy
(818) 356-4319 02-2 $76,500

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

## CARNEGIE MELLON UNIVERSITY
**Pittsburgh, PA 15213-3890**

**252. PRESSURE-INDUCED AMORPHIZATIONS OF SILICON ANALOGUES: A PROBE OF THE RELATIONSHIP BETWEEN ORDER AND DISORDER**
W.S. Hammack, Department of Chemical Engineering
(412) 268-2227 01-1 $90,000

Pressure induced amorphization of silica analogues. Determination of medium range order in amorphous solids. In-situ Raman and X-ray diffraction at high pressure and post transformation HRTEM. The role of topology, ionicity and packing in the crystalline to amorphous transformation.

**253. THE EFFECTS OF APPLIED STRESS ON MICROSTRUCTURAL EVOLUTION**
W. C. Johnson, Department of Materials Science and Engineering
(412) 268-8785 01-1 $86,768

Theoretical and computer simulation of microstructural evolution of two-phase systems under stress. The influence of misfit strains and external stress on precipitate shape, size and distribution. Computer simulation predicting particle alignment, and inverse coarsening during Ostwald ripening.

**254. THE ROLE OF MICROSTRUCTURAL PHENOMENA IN MAGNETIC THIN FILMS**
D. E. Laughlin, Department of Metallurgical Engineering
(412) 268-2706

D. N. Lambeth, Department of Electrical and Computer Engineering
(412) 268-3674 01-1 $83,600

Effects of microstructure of thin magnetic films on extrinsic magnetic properties. Systematic variation of important microstructural features, such as grain size and crystallographic texture, by control of variables used during processing. Interrelationship of microstructure, magnetic domain structure and extrinsic magnetic properties of magnetic thin films will be determined.

**255. INVESTIGATIONS OF THE INTERPLAY BETWEEN COMPOSITION AND STRUCTURE AT INTERPHASE BOUNDARIES**
P. Wynblatt, Department of Materials Science and Engineering
(412) 268-8711 01-1 $91,106

Combined experimental and theoretical study of the relation between composition and structure of solid/solid interphase boundaries. Experimental approaches include: solid state wetting studies of one phase by another, atomic resolution electron microscopy of interfacial structure, and atom-probe field ion microscopy of interfacial composition. Systems to be studied include Pb-Cu doped with Ag and Au, Cu-Ag doped with Au, and possibly Pb-Ni with appropraite dopants. Modelling of interphase boundary structure and composition will be performed by Monte Carlo techniques.

## UNIVERSITY OF CHICAGO
**5640 Ellis Avenue**
**Chicago, IL 60637**

**256. HIGH-TEMPERATURE THERMOCHEMISTRY OF TRANSITION METAL BORIDES AND SILICIDES**
O. J. Kleppa, The James Franck Institute
(312) 702-7198 01-3 $52,060

Detailed experimental study of transition metal silicides and borides using solute-solvent drop calorimetry, a technique which provides experimental access to the thermochemistry of a wide range of refractory materials. Establish systematic trends in the enthalpy of formation for transition metal silicides and borides.

## UNIVERSITY OF CINCINNATI
**Cincinnati, OH 45221**

**257. ROLE OF INTERFACIAL PROPERTIES ON THE STEADY STATE AND NON-STEADY STATE FIRST-MATRIX CRACKING BEHAVIORS IN CERAMIC-MATRIX COMPOSITES**
R. N. Singh, Department of Materials Science and Engineering
(513) 556-3119 01-5 $120,400

Study of the steady state and non-steady state first-matrix cracking behaviors in fiber-reinforced ceramic composites. Fabricate composites with tailored microstructure, flaw size, fiber architecture, and interfacial properties. Establish the role of interfacial properties and flaw size on the first-matrix cracking behavior in the steady state and non-steady state matrix cracking regimes.

## CITY UNIVERSITY OF NEW YORK AT CITY COLLEGE
**New York, NY 10031**

**258. DYNAMICS AND PATTERN SELECTION AT THE CRYSTAL-MELT INTERFACE**
H. Z. Cummins, Department of Physics
(212) 690-6921 02-2 $108,000

Dynamics at the crystal-melt interface, especially the initial instability and growth of small fluctuations in the linear regime, evolution of the pattern through the nonlinear coarsening stage, restabilization and continuous sidebranching. Morphological instability and pattern selection in which a uniform featureless volume or smooth interface spontaneously destabilizes and evolves to form a complex spatial pattern as in a crystal growing into its undercooled melt.

**259. MAGNETIC PROPERTIES AND CRITICAL BEHAVIOR OF THE CONDUCTIVITY NEAR THE M-I TRANSITION**
M. P. Sarachik, Department of Physics
(212) 690-6904 02-2 $85,000

Investigation of the transport and dielectric properties of doped semiconductors which undergo a transition from insulating to metallic behavior with increasing dopant concentration. Examination of the role of disorder and correlations on the transition. Determination of the effect of spin-orbit scattering, spin-flip scattering, magnetic field and quantum interference phenomena. Experiments will include measurements of resistivity, Hall coefficient and dielectric constant of n-type CdSe and of uncompensated and compensated Si:B using uniaxial stress in varying magnetic fields.

**260. TRANSPORT IN SMALL AND/OR RANDOM SYSTEMS**
M. Lax, Department of Physics
(212) 690-6864 02-3 $109,250

Theoretical research on electron and hole transport in quasi-2D systems including the interaction of hot phonons. Time-dependent effects down to the femtosecond regime, strong and/or microwave fields and negative resistance effects are considered. Resonance tunneling assisted by phonon relaxation and infrared radiation are explored. Fundamentals of semiconductor laser operation are reexamined and partial noise in the presence of feedback is evaluated.

## CITY UNIVERSITY OF NEW YORK AT QUEENS COLLEGE
**Flushing, NY 11367**

**261. OPTIMAL SYNTHESIS OF NEW RARE EARTH TRANSITION METAL PERMANENT MAGNET SYSTEMS**
F. J. Cadieu, Department of Physics
(718) 997-3609 01-1 $67,559 (24 months)

Synthesis and study of new rare earth transition metal permanent magnet systems. This consists of elucidating the sputter process growth dynamics which allow specifically-textured magnetic films of different systems to be synthesized, and fabricating layered structures utilizing systems with in-plane and perpendicular-to-the-plane magnetic anisotropies.

**262. DETERMINATION OF CONCENTRATION PROFILES AT INTERFACES AND SURFACES OF PARTIALLY MISCIBLE POLYMER BLENDS**
M. Rafailovich, Department of Physics
(718) 997-3385

J. Sokolov, Department of Physics
(718) 997-3385 03-2 $66,696

This program studies the form of the surface and interfacial profiles in model blends of chemically different polymers with varying levels of miscibility; highly immiscible deuterated polystyrene/polystyrene-co-bromostyrene (dPS/PBr$_x$S), for large degree of bromination, x, and polymerization index, N, and nearly compatible $d_3$PS/PS or $d_5$PS/PS blends where $d_3$ and $d_5$ refer to backbone and side-group deuteration, respectively. The experimental program will systematically explore the equilibrium properties of the profiles as functions of temperature, chain length, degree of bromination, segment deuteration and blend composition. The profiles will be determined by several complementary techniques: (a) Secondary Ion Mass Spectrometry (SIMS), (b) Forward Recoil Elastic Scattering (FRES) with simultaneous measurement of time-of-flight and energy (TOF-FRES), (c) neutron and

X-ray reflectivity (NR, XR) and (d) X-ray fluorescence under conditions of near-total external reflection (NTEF). This will enable us to obtain for the first time unique solutions to the concentration profiles, which will form the experimental basis for critical discrimination between current molecular theories.

## CLARK ATLANTA UNIVERSITY
**223 J.P. Brawley Drive, SW**
**Atlanta, GA 30314-4381**

**263. THE SYNTHESIS, CHARACTERIZATION AND CHEMISTRY OF SI-C-N-O-M CERAMIC AND COMPOSITE POWDERS**
Y. H. Mariam, Department of Chemistry
(404) 880-8593 01-3 $58,772

Preparation of Si-C-N-O-M/Si-C-N-M systems, where M=Ti or Zr, from silazane/organosilylamine polymer precursors. Molecular and chemical structures, microstructures, composition, morphology and microcrystallinity of powders investigated by SEM, TEM, EXAFS, EXELFS, etc. Detailed nitridation followed by physical- and chemical state characterization. Computational modeling of certain reactions relevant to nitridation, decomposition and cross-linking performed using semiempirical molecular orbital methods to obtain reaction enthalpies, activation enthalpies and entropies, and potential energy surfaces. Modeling studies coupled with TGA/FTIR, decomposition kinetics, evolved gas analysis to investigate role of chemical reactivity and structure in formation chemistry of ceramic and composite powders.

## COLORADO SCHOOL OF MINES
**Golden, CO 80401**

**264. NOVEL CONCEPTS IN WELD METAL SCIENCE: ROLE OF GRADIENTS AND COMPOSITE STRUCTURE**
D. L. Olson, Center for Welding and Joining Research
(303) 273-3775

D. K. Matlock, Center for Welding and Joining Research
(303) 273-3775 01-5 $105,600

Composite modeling techniques, applied previously to describe the effects of compositional and microstructural gradients on weld metal properties in austenitic alloys, extended to the analysis of several new weld metal systems of interest for joining new materials. Systems of interest include composites of a soft weld metal with insoluble hard second phase particles or alternating deformable phases of approximately equal volume fractions. Special techniques to produce laboratory samples with microstructures which simulate the composition and microstructure gradients in solidified weld metal. Appropriate mathematical models to evaluate the properties of the composite weld metals.

**265. POTENTIAL MODULATION OF EQUILIBRIUM AND EXCITATION PHENOMENA AT THE ELECTROLYTE-SOLID INTERFACE**
T. Furtak, Department of Physics
(303) 273-3843 02-2 $85,000

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

## COLUMBIA UNIVERSITY
**New York, NY 10027**

**266. PROTONS AND LATTICE DEFECTS IN PEROVSKITE-RELATED OXIDES**
A. S. Nowick, Krumb School of Mines
(212) 854-2921 01-3 $117,040

Defect chemistry of pure and doped perovskite-related oxides that include $KTaO_3$, $BaCeO_3$, $CaTiO_3$, and mixed order/disorder type perovskites. Utilization of EPR and IR techniques, in addition to electrical conductivity and dielectric relaxation measurements. Deuteron NMR measurements in deuterium-charged samples to study the interaction of deuterons with other deuterons and the lattice. Computer simulation techniques to study and predict defect-dopant behavior. Study of the Jonscher "universial" relaxation effect in simple ionic materials over a wide temperature regime.

## UNIVERSITY OF CONNECTICUT
**Storrs, CT 06268**

**267. TRANSFORMATION TOUGHENING**
P. C. Clapp, Department of Metallurgy
(203) 486-4714 01-1 $130,337

Development of a theory of transformation toughening that includes the contribution of the shear components of the trnasformation strain and the precise details of the location of stress induced martensitic nucleation in the stress field around a propagating crack tip and the non-isotropic and non-linear elastic effects. A number of previous efforts have used continuum elasticity theory, but all ignore the effects of the shear components of the martensitic transformation, assume that the transformation is nucleated purely by the hydrostatic component of the stress field, and take essentially no account of any non-linear elastic effects.

**268. SYNCHROTRON RADIATION STUDIES OF LOCAL STRUCTURE AND BONDING IN HIGH TC SUPERCONDUCTING OXIDES, TRANSITION METAL ALUMINIDES AND SILICIDES**

J. I. Budnick, Department of Physics
(203) 486-5541 02-2 $80,000

Explore local structural properties in a variety of superconducting oxide systems and their relevance: to the understanding of the doping mechanism and local atomic and electronic structure, the synthesis of new superconducting materials; to the mechanical properties of both binary transition metal aluminides and the role of small ternary additions which can enhance ductility; to the ability to improve Curie temperatures and magnetic anisotropy by nitriding systems such as $Sm_2Fe_{17}$; and to the understanding of the evolution of complex silicides.

## CORNELL UNIVERSITY

**120 Day Hall**
**Ithaca, NY 14853-2801**

**269. THEORY OF NONLINEAR, DISTORTIVE PHENOMENA IN SOLIDS: MARTENSITIC, CRACK AND MULTISCALE STRUCTURES-PHENOMENOLOGY AND PHYSICS**

J. A. Krumhansl, Department of Physics
(607) 255-5261

J. P. Sethna, Department of Physics
(607) 255-5261 01-1 $138,829

Development of a general theoretical framework for analyzing displacive changes and application to a few selected martensitic transformations. Physics of transformation, mesostructure, and cracking by large lattice distortion. "Tweed" precursor textures in martensitic materials several hundred degrees above their bulk transformation temperatures. Continuum theory for brittle crack growth in three dimensions. Broad search for giant elastic softening, glassy low temperature properties, and nucleation and nucleation dynamics.

**270. STUDIES OF THE III-V COMPOUNDS IN THE MEGABAR REGIME**

A. L. Ruoff, Department of Materials Science and Engineering
(607) 255-4161 01-1 $113,666

Crystal structure of III-V compounds with low atomic number as a function of pressure to 200-300 GPa (2-3 Mbar) with emphasis on transformations from four-fold to six-fold, eight-fold and twelve-fold coordination. Metallic properties characterized by visible and near infrared reflectivity. Verification of theoretical models using broad range of pressure, coordination number, and interatomic spacing.

**271. EXPERIMENTAL STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES**

S. L. Sass, Deparment of Materials Science and Engineering
(607) 255-5239 01-1 $160,706

Investigation of the structure and chemistry of grain boundaries in $Ni_3AL$ and NiAl in the presence and absence of boron. Influence of solute-induced changes in the structure of grain boundaries on their mechanical properties. Study of the possibility of control of mechanical properties of ceramic grain boundaries. Techniques include transmission electron microscopy, Auger electron spectroscopy, electron diffraction, and X-ray diffraction techniques.

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

J. Silcox, School of Applied and Engineering Physics
(607) 255-3332

E. J. Kirkland, School of Applied and Engineering Physics
(607) 255-3332 01-1 $113,666

Compound formation between silicon and heavy transition elements and grain boundaries in $Ni_3Al$ studied by annular dark field scanning transmission electron microscopy (ADF-STEM) at atom structure resolution level and other analytical electron microscopic methods. Initial stages of epitaxial elemental or silicide thin film formation in early cluster formation, island, surface domain and interface formation on silicon. Effects of annealing and contaminant gases (e.g., $O_2$, $H_2$) on observed structures. Structure, chemical composition and local electronic structure of grain boundaries in $Ni_3Al$ determined with annular dark field Z-contrast, convergent beam electron diffraction and electron energy loss spectroscopy.

**273. CERAMIC FILMS AND INTERFACES: CHEMICAL AND MECHANICAL PROPERTIES**
Rishi Raj, Department of Materials Science and Engineering
(607) 255-4040 01-2 $155,434

Research on structure and composition of interfaces between dissimilar ceramics and on correlation between structure, chemistry and mechanical properties. The investigation will use alumina/zirconia interfaces in layered thin films under controlled oxygen partial pressures. There is special emphasis on the formation of intergranular phases. Structure will be characterized by high resolution TEM, chemistry by scanning TEM, and mechanical properties by internal friction, fracture, and plasticity behavior.

**274. SURFACE PHASES AND THEIR INFLUENCE ON METAL-OXIDE INTERFACES**
J. M. Blakely, Department of Materials Sciences and Engineering
(607) 255-5149 01-3 $99,231

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

**275. DEFECTS AND TRANSPORT IN MIXED OXIDES**
R. Dieckmann, Department of Materials Science and Engineering
(607) 255-4315 01-3 $98,120

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

**276. THE GEOMETRY OF DISORDER: THEORETICAL INVESTIGATIONS OF QUASICRYSTALS AND FRUSTRATED MAGNETS**
C. L. Henley, Department of Physics
(607) 255-5056 02-3 $35,000 (9 months)

Investigation of quasicrystal geometry to compute phason elastic constants, investigation of quasicrystal atomic structure fitting data to atomic model of a decorated cell and cluster packing, and develop structure models for all decagonal phases. Determine in randomly frustrated spin systems with carrier spin interactions, the "spin-glass" insulating phase of high-$T_c$'s, the excited states of the hole-spin and in classical Cu:Mn spin glasses propose new experimental tests for "spin-density wave" and "Fermi-liquid" pictures. In percolation and nonlinear dynamics, determine, analytically, the exponents of the self-organized percolation model in one dimension and in mean field theory.

**277. SYNTHESIS AND PROPERTIES OF NOVEL CLUSTER PHASES**
F. J. DiSalvo, Department of Chemistry
(607) 255-7238 03-1 $162,106

Synthesis of new cluster compounds, Chevrel phases, containing the metals, Nb, Ta, Mo, W and Re. Compounds are usually halides, chalcogenides, oxides or pnictides. Examination of solid state synthesis and properties of new metal cluster chalcogenide phases to be emphasized. Synthesis to exploit some of the known solution chemistry of halide compounds to obtain novel kinds of compounds. Properties such as: superionic conductivity, very high superconducting magnetic behavior and thermally induced valence transitions of post-transition elements to be determined. Study of $Mo_3X_3$ infinite chain clusters and polymer blends of these inorganic polymers with organic polymers. Synthesis of complexes of $Nb_6I_8$ with bifunctional ligands or with square planar metal organic or coordination complexes. Characterization by X-ray diffraction, Faraday balance for magnetic measurements, four probe resistance for conductivity, Hall effect, and magneto-resistance measurements.

## DARTMOUTH COLLEGE
**Hanover, NH 03755**

**278. THE HALL-PETCH RELATIONSHIP AND MECHANISMS OF FRACTURE IN B2 COMPOUNDS**
I. Baker, Thayer School of Engineering
(603) 646-2184 01-2 $82,431

An investigation of the relationship between the parameter K, in the Hall-Petch Relationship, $\alpha_y = \alpha_o + Kd^{-1/2}$, and grain boundary structure/chemistry in a number of $B_2$ compounds. Grain boundary structure and chemistry determined by scanning transmission electron microscopy and Auger electron microscopy. Grain boundary dislocation structures examined by transmission electron microscopy including in-situ straining experiments. Slip trace analysis of polished surfaces to examine planarity of slip. Fracture modes determined by scanning electron microscopy. Extent of plastic deformation on fracture surfaces determined by selected area channelling patterns.

**279. THE NOTCH SENSITIVITY OF INTERMETALLIC COMPOUNDS**

E. M. Schulson, Thayer School of Engineering
(603) 646-2888 01-2 $113,721

Intermetallic compounds; notch sensitivity and relationship to work hardening; B-doped Ni-rich $Ni_3Al$, $Zr_3Al$, $Ni_3FE$ and B-doped single crystals of $Ni_3Al$; effects of triaxiality of stress state, strain rate, temperature, environment, prestrain and orientation of single crystals; near-notch tip deformation field through microhardness and through optical, transmission and scanning electron microscopy.

## UNIVERSITY OF DELAWARE
**Newark, DE 19716**

**280. FUNDAMENTAL STUDIES OF NEW HIGH ENERGY PERMANENT MAGNET MATERIALS**

G. C. Hadjipanayis, Department of Physics
(302) 451-2661 02-2 $45,800

Research to advance the understanding of new, strongly magnetic rare earth-transition metal compounds and alloys. Magnetic phases studied are based on iron and light rare earths, and are generally ternary or higher order alloys with unusually complex, anisotropic structures. The type of systems investigated include new Fe-rich phases which are nitrogenated or carbonated to enhance their magnetic properties, new phases reached by intermediate metastable phases via melt spinning, and sputtered thin films and multilayers. Comprehensive experiments include X-ray and neutron diffraction, electron microscopy, dc and ac magnetic susceptibilities, Mossbauer spectroscopy, and photoemission. Experimental results compared with spin-polarized, self-consistent electronic structure calculations. Research performed in close collaboration with work at the University of Nebraska.

## FLORIDA ATLANTIC UNIVERSITY
**Boca Raton, FL 33431**

**281. THEORETICAL STUDIES OF METALLIC ALLOYS**

J. S. Faulkner, Department of Physics
(407) 367-3429 01-1 $96,628 (18 months)

Techniques for total energy calculations developed within the framework of the KKR-CPA and the non-muffin tin quadratic KKR (QKKR) band theory method. The energies, $Ex(K_j)$, calculated from the embedded cluster method (ECM) and the energies of the ordered phases will be obtained with the QKKR. Realistic first principles calculations of phase diagrams and phase stability parameters will then be performed on the alloys such as PdRh, CuPd, PdRh, CuAu and other topical systems.

## FLORIDA STATE UNIVERSITY
**Tallahassee, FL 32306**

**282. HEAVY FERMIONS AND OTHER HIGHLY CORRELATED ELECTRON SYSTEMS**

P. U. Schlottmann, Department of Physics
(904) 644-0055 02-3 $58,202 (9 months)

Theoretical investigation of highly correlated fermion systems. The Bethe-ansatz is used to solve the orbitally degenerate Anderson impurity model with finite Coulomb repulsion. The dynamics of the n-channel Kondo problem is investigated within a 1/n expansion. The thermodynamic Bethe-ansatz equations of the n-channel Kondo problem are solved numerically in a magnetic field. The low temperature and small field magnetoresistivity of heavy-fermion alloys is studied. The properties of the spin-one Heisenberg chain with anisotropies induced by crystal fields and the generalized t-J model in one and two dimensions are investigated.

**283. HE-ATOM SURFACE SCATTERING: SURFACE DYNAMICS OF INSULATORS, OVERLAYERS AND CRYSTAL GROWTH**

J. G. Skofronick, Department of Physics
(904) 644-5497

S. A. Safron, Department of Chemistry
(904) 644-5239 02-4 $70,000 (7 months)

Application of a He atom-surface scattering instrument to the investigation of surface dynamics of ionic insulators including MgO, NiO, KCN, and perovskites. Continued investigations of epitaxial growth as a function of growth parameters and molecular size. Examination the dynamics of the head groups of alkyl thiols which self-assemble on Au and Ag. Investigation of the surface magnetic properties of magnetic superlattices such as $NiO/Fe_3O_4$ prepared by molecular beam epitaxy. Temperature dependent multiphonon measurements on all systems will be made.

## UNIVERSITY OF FLORIDA
**Gainesville, FL 32611**

**284. X-RAY SCATTERING STUDIES OF NON-EQUILIBRIUM ORDERING PROCESSES**
S. E. Nagler, Department of Physics
(904) 392-8842 02-2 $59,000

Investigation of the kinetics of first order phase transitions. Time resolved high resolution X-ray scattering is used to probe development of order in materials that have been rapidly quenched through a phase transition. Synchrotron radiation measurements complement in-house experiments using a rotating anode. Systems under investigation include thin films and single crystals of alloys, block co-polymers, and the martensitic transformation in solid hydrogen. Emphasis is on elucidating the underlying universal features of the kinetics.

**285. STUDIES OF NOVEL SUPERCONDUCTORS**
G. R. Stewart, Department of Physics
(904) 392-9263 02-2 $85,000

Experimental investigations will be made on "heavy-Fermion" systems with emphasis on possible new "super-heavy systems such as $CePt_2Sn_2$ and YbBiPt; dilute $U_{1-x}M_xPt_3$; hydrogen doped heavy-Fermion systems; and new Np and Pu intermetallics. These compounds will be obtained or prepared and characterized by techniques including X-ray diffraction, resistivity, dc and ac susceptibility and specific heat.

## GEORGIA TECH RESEARCH CORPORATION
**Atlanta, GA 30332-0430**

**286. FIRST-PRINCIPLES STUDIES OF PHASE STABILITY AND THE STRUCTURAL AND DYNAMICAL PROPERTIES OF METAL HYDRIDES**
M. -Y. Chou, Department of Physics
(404) 894-4688 02-3 $42,500

Problems to be investigated include: disorder-disorder, disorder-order and order-order phase transitions found in the temperature-composition diagrams; preferential interstitial sites of hydrogen in different metals, the change of optimal sites under hydrogen in different metals, the change of optimal sites under static pressure or uniaxial stress; the vibrational spectra, diffusion barrier and migration path of hydrogen in metals. Structural and electronic properties will be examined by total-energy calculations for a series of metal hydrides by the local-density-functional approximation and the pseudopotential method. Various hydrogen concentrations and configurations will use the supercell methods. Within the framework of cluster expansions, the multibody interaction energies among hydrogen atoms as extracted from the total energies of related ordered structures are used to investigate the thermodynamic properties and phase diagrams by the cluster variational method.

**287. STRUCTURE AND DYNAMICS OF MATERIAL SURFACES, INTERPHASE-INTERFACES AND FINITE AGGREGATES**
U. Landman, School of Physics
(404) 894-3368 02-3 $206,000

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

**288. GROWTH, STRUCTURE AND STABILITY OF EPITAXIAL OVERLAYERS**
A. Zangwill, Department of Physics
(404) 894-7333 02-3 $73,000

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

**289. THE ORGANIC CHEMISTRY OF CONDUCTING POLYMERS**
L. M. Tolbert, Department of Chemistry
(404) 894-4043 03-1 $82,500

The phenomenon of charge transport in conducting polymers, materials which are ordinarily insulators, is basically a problem in mechanistic organic chemistry. Fundamental studies in the mechanistic organic chemistry of conducting polymers are being conducted. Oligomers of defined length have been synthesized, and a comparison of their spectroscopic properties as they converge with those of the associated polymers is being carried out. This approach has allowed a validation of solid state theory. New alternating heteropolymers which have enhanced stability and processability, while retaining the desirable characteristics of more well-known polymers such as polythiophene, are being synthesized. This novel class of heteropolymers is characterized by strong charge-transfer characteristics and significantly smaller band gaps than the hompolymers.

## UNIVERSITY OF GEORGIA
**Athens, GA 30602**

**290. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS**
W. M. Yen, Department of Physics and Astronomy
(404) 542-2491 02-2 $75,000 (9 months)

Investigation of relaxation, transfer and quenching of the excited states of disordered materials; nonlinear optical properties and structure of activated glass fibers and their elementary excitations; and extremely diluted and single ions in disordered systems. Application of advanced laser techniques, including fluorescence line narrowing (FLN) and time-resolved FLN, Dilution Narrowed Laser Spectroscopy (DNLS), Saturation Resolved Fluorescence Spectroscopy (SRF), measurement of coherent optical transients, photoacoustic and photocaloric methods, and far infrared free electron laser.

## HARVARD UNIVERSITY
**29 Oxford Street**
**Cambridge, MA 02138**

**291. SOLUTE TRAPPING AND EFFECTS ON SOLIDIFICATION MICROSTRUCTURES**
M. J. Aziz, Division of Applied Science
(617) 495-9884 01-1 $79,200

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

**292. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS**
I. F. Silvera, Department of Physics
(617) 495-9075 02-2 $150,000 (9 months)

Investigation of the properties of quantum gases of spin-polarized atomic hydrogen and deuterium. Attempt to reach sufficient densities and low temperatures that these unusual gases will undergo Bose-Einstein condenstion using one or more of four approaches: self compression of hydrogen to high density in micron sized bubbles of helium; isolating hydrogen from van der Waals walls in a hybrid static/microwave magnetic trap, in conjunction with laser cooling and diagnostics; cooling of a two dimensional gas of hydrogen in an inhomogeneous magnetic field; and compression of spin-polarized hydrogen in a bubble with spin-polarized electrons on the surface.

**293. SYNCHROTRON STUDIES OF X-RAY REFLECTIVITY FROM SURFACES**
P. S. Pershan, Division of Applied Sciences
(617) 495-3214 03-3 $69,000

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

## UNIVERSITY OF HOUSTON
**Houston, TX 77004-5506**

**294. DIFFRACTION STUDIES OF THE STRUCTURES OF GLASSES AND LIQUIDS**
S. C. Moss, Department of Physics
(713) 749-2840 02-1 $125,600 (17 months)

Development and operation of a dedicated glass and liquid neutron diffractometer (GLAD) for use at the Intense Pulsed Neutron Source (IPNS) of Argonne National Laboratory with support and collaboration from Argonne. Investigations of the structure of glasses and liquids by X-ray and neutron scattering methods. Laser light scattering studies of colloidal and polymeric systems.

## IBM
**650 Harry Road**
**San Jose, CA 95120-6099**

**295. SEGMENTAL INTERPENETRATION AT POLYMER-POLYMER INTERFACES**
T. P. Russell, Almaden Research Center
(408) 927-1638 03-2 $103,703

The behavior of block copolymers at interfaces will be studied with the use of neutron and X-ray reflectivity, XPS, dynamic SIMS (DSIMS), and forward recoil specrometry (FRES). The subjects of investigation will include the behavior of diblock copolymer in confined geometries, the interfacial behavior of the symmetric diblock copolymer, P(S-b-MMA) at the interface between PS and PMMA homopolymers, the interfacial behavior of multiblock copolymers, and the behavior of diblock copolymers at the interface of dissimilar hompolymers. The combined use of the four techniques mentioned above, coupled with small angle X-ray and neutron scattering, will permit a quantitative evaluation of the segment density profiles of block copolymers at interfaces and will allow a critical assessment of current theoretical treatments of the interfacial behavior of block copolymers.

## INDIANA UNIVERSITY
**Bloomington, IN 47405**

**296. HIGH-RESOLUTION ELECTRON ENERGY LOSS STUDIES OF SURFACE VIBRATIONS**
L. Kesmodel, Department of Physics
(812) 855-0776 02-2 $110,107

Investigation of surface vibrational properties on metal surfaces, ultrathin magnetic films, semiconductor and metal-semiconductor systems using high-resolution electron energy loss spectroscopy (EELS) with an energy resolution of 3-5 meV. Detailed surface phonon dispersion information to be obtained on copper, silver, iron, iron/silver and aluminum/silicon with and without adsorbates such as hydrogen, oxygen, and sulfur. Results to be compared with realistic theoretical models of surface lattice dynamics and inelastic electron scattering.

## JOHNS HOPKINS UNIVERSITY
**105 Ames Hall**
**Baltimore, MD 21218**

**297. INVESTIGATION OF THE PROCESSES CONTROLLING THE FLAME GENERATION OF REFRACTORY MATERIALS**
J. L. Katz, Department of Chemical Engineering
(410) 516-8484 01-3 $65,076

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

**298. CRITICAL ISSUES IN DE-ALLOYING AND TRANSCRYSTALLINE STRESS-CORROSION CRACKING**
K. Sieradzki, Department of Materials Science and Engineering
(410) 516-5409

J. W. Wagner, Department of Materials Science and Engineering
(410) 516-5409 01-5 $70,400

Research addresses three major areas: a) the dynamics of the film-induced micro-cleavage process; b) the effect of the electrochemical potential on the coarsening of de-alloyed sponges and c) the mechanical properties of de-alloyed layers. Test parameters include de-alloyed film thickness, foil texture, electrochemical potential, dynamic displacement rates and amplitude of the applied displacement. The role of the penetrate into ductile substrate will be examined. The propagation of brittle elastic cracks in a 10 micron thick foil coarsening of de-alloyed layers will be measured by: a) electrochemical techniques, b) grazing angle X-ray scattering and X-ray reflectivity measurements at NSLS and c) scanning tunneling microscopy. The effect of coarsening on the elastic and fracture properties of the layers will also be measured. Alloy systems include Zn-Cu, Ag-Au and Cu-Au.

## LEHIGH UNIVERSITY
**Bethlehem, PA 18015**

**299. ANALYTICAL ELECTRON MICROSCOPY OF BIMETALLIC CATALYSTS**
C. E. Lyman, Department of Metallurgy and Materials Engineering
(215) 758-4220 01-1 $84,063

Elucidation of structure-property relationships in platinum-rhodium bimetallic catalyst for NOx reduction. Measurement of the distribution of noble metal and catalytic poisons on a micrometer to nanometer scale by electron beam microanalytical methods. Correlation of catalyst microstructure with catalytic activity and selectivity. Impregnation procedure leading to different noble metal distributions, oxidation and reduction of NOx in hydrogen.

**300. HIGH RESOLUTION MICROSTRUCTURAL AND MICROCHEMICAL ANALYSIS OF ZIRCONIA EUTECTIC INTERFACES**
M. R. Notis, Department of Metallurgy and Materials Sciences
(215) 758-4225 01-1 $102,551

Eutectic interfaces studied in as-grown $MnO-ZrO_2$, $NiO-ZrO_2(Y_2O_3$, $CoO-ZrO_2(CaO)$, and $NiO-Y_2O_3$ systems. High resolution microstructural and microanalytical methods (HRTEM, CBED and PEELS) used to study interfaces in plan-view and conventional configurations. Local oxidation state across grain boundaries in single phase MnO and MnO-$ZrO_2$ studied as function of oxygen partial pressure. Segregation effects due to ternary additions measured at interphase interfaces and at local defects and faults within interfaces.

**301. THE EFFECT OF POINT DEFECTS AND DISORDER ON STRUCTURAL PHASE TRANSITION**

J. Toulouse, Department of Physics
(215) 758-3960 01-1 $52,061

Dielectric, ultrasonic and Raman spectroscopic investigation of point defect-soft mode coupling and the effect of defects on critical fluctuations of phase transitions in fluoroperovskites and oxyperovskite having either a zone center or a zone boundary mode. Extension of frequency and concentration range in study of two model systems: $KTa_{1-x}Nb_xO_3$ (KTN), zone center mode; and $KZnF_3$:Li and $KMnF_3$:Li, zone boundary mode. Investigation of effects of defects in $KTaO_3$:Li, where Li substitutes off-center for K, and in $KMnF_3$:Na, Ca, where Na and Ca substitute for on-center. Origin of diffuse character of phase transitions studied in KTN and "relaxor" systems; characterization of low-temperature "dipolar glass" behavior of these materials. Investigation of soft mode behavior in mixed systems for which end members have different types of soft mode condensation to attain understanding of condensation process and morphotropic phase boundary behavior.

**302. CORROSION FATIGUE OF IRON-CHROMIUM-NICKEL ALLOYS: FRACTURE MECHANICS, MICROSTRUCTURE AND CHEMISTRY**

R. P. Wei, Department of Mechanical Engineering and Mechanics
(215) 758-3585 01-2 $113,102

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

**303. ROLE OF STRUCTURE ON ION MOVEMENT IN GLASSES**

H. Jain, Department of Materials Science and Engineering
(215) 758-4217 01-3 $52,800

Investigation of the correlation and dependence of ion motion in glasses on local structure. Structure of selected glasses modified by both thermal and radiation treatments and characterized using NMR and IR/Raman spectroscopies. Localized ion motion characterized by dielectric and nuclear-spin relaxation. Long range ion movement characterized by dc conductivity and tracer diffusion measurements.

## LOUISIANA STATE UNIVERSITY
**Baton Rouge, LA 70803-4001**

**304. EMBEDDED MICROCLUSTERS IN ZEOLITES AND CLUSTER BEAM SPUTTERING - SIMULATION ON PARALLEL COMPUTERS**

P Vashishta, Computer Laboratory for Materials Simulation
(504) 388-1157

R Kalia, Computer Laboratory for Materials Simulation
(504) 388-1157 02-3 $59,000 (18 months)

Computer simulation studies of (1) atoms and microclusters embedded in zeolites and (2) the sputtering of insulating and semiconducting surfaces by a variety of atomic, ionic, and cluster beams. Simulation approaches include classical molecular dynamics, Car-Parrinello, quantum molecular dynamics, and variational quantum Monte Carlo. Research incorporates studies of techniques to determine realistic interaction potentials and algorithm development for massively parallel computer architecture. The work on embedding of zeolites includes investigation of both the zeolite networks and the isolated microclusters before embedding. Embedding species include individual atoms (e.g., Si, S, and Te), binary molecules (e.g., GaAs,InSb, PbSe, $SiO^2$, $GeSe^2$, and SiC), and clusters of the indicated atoms and molecules. Some of the sputtering simulations involve Si surfaces bombarded by charged and neutral Si clusters, GaAs and InSb surfaces by a variety of cluster beams, erosion of LiF surfaces by NaCl and $CaF^2$ clusters, and sputtering of solid C by $H^2O$ clusters.

## UNIVERSITY OF MAINE
**Orono, ME 04469**

**305. STRUCTURE, ADHESION, AND STABILITY OF METAL/OXIDE AND OXIDE/OXIDE INTERFACES**
R. J. Lad, Department of Physics
(207) 581-2257 01-1 $67,760

Fundamental properties of metal/oxide and oxide/oxide heterogeneous interfaces with emphasis on effects of interfacial defects, impurities, carbon layers, and amorphous phases on interfacial morphology, adhesion, electronic structure, and high temperature stability. Deposition of ultra-thin metal and oxide films (viz. Al, Fe, Cu, $Al_2O_3$, $Fe_xO$, CuO, and $SiO_2$) on single crystal $TiO_2$ and NiO substrates. Determination of film epitaxy and interface morphology by in-situ RHEED analysis and Atomic Force Microscopy; determination of composition, chemical bonding, interdiffusion, segregation and electronic structure information by X-ray and ultraviolet photoemission, Auger spectroscopy, and EELS.

## MASSACHUSETTS INSTITUTE OF TECHNOLOGY
**77 Massachusetts Avenue**
**Cambridge, MA 02139**

**306. GRAIN BOUNDARIES**
R. W. Balluffi, Department of Materials Sciences and Engineering
(617) 253-3349

P. D. Bristowe, Department of Materials Sciences and Engineering
(617) 253-3326 01-1 $454,960

Studies of the atomic structure of grain boundaries, with and without segregated solute atoms, by X-ray diffraction and computer simulation. Grain boundary diffusion and its dependence on boundary structure by combined experimental observations and computer simulation. Computer simulation of grain boundary migration. Materials studied include Au, Au containing Mg solute atoms, Ag, and Si. Experimental techniques include X-ray diffraction at the NSLS and high-resolution and conventional electron microscopy. Computer simulation. Embedded Atom Model.

**307. DETERMINISTIC ANALYSIS OF PROCESSES AT CORRODING METAL SURFACES AND THE STUDY OF ELECTROCHEMICAL NOISE IN THESE SYSTEMS**
R. M. Latanision, Department of Materials Science and Engineering
(617) 253-4697 01-1 $65,076

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

**308. GRAIN BOUNDARIES IN MULTICOMPONENT CERAMICS**
Y-M. Chiang, Department of Materials Science and Engineering
(617) 253-6471 01-2 $95,444

Investigation of grain boundary nonstoichiometry and its relation to grain boundary mobility, diffusional creep mechanisms/rates, and electrical properties. Materials studied include titanium oxide, strontium/barium titanates, and the superconducting cuprates. Correlation of grain boundary stoichiometry and composition, as determined by STEM light-element microanalysis and Auger spectroscopy, with the electrical property behavior that is determined by DC electrical conductivity and AC complex impedance analyses.

**309. STRUCTURAL DISORDER AND TRANSPORT IN TERNARY OXIDES WITH THE PYROCHLORE STRUCTURE**
H. L. Tuller, Department of Materials Science and Engineering
(617) 253-6890 01-3 $116,768

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

**310. MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS**

J. B. Vander Sande, Department of Materials Science and Engineering
(617) 253-6933 01-3 $164,502

Processing of superconducting oxide/Ag microcomposites by oxidation of metallic precursor alloys including microstructural characterization and electrical property measurements of product phases generated, with emphasis on $YbBa_2Cu_3O_x$/Ag and $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$/Ag. In addition to specific work on the formation, structure, and properties of superconducting oxide/Ag microcomposites, research is underway on the development of texture by solid state thermal gradient processing to produce textured superconducting oxides at high growth rates and development of models for, and experiments on, combustive oxidation including work on model systems.

**311. RADIATION-INDUCED APERIODICITY IN IRRADIATED CERAMICS**

L. W. Hobbs, Department of Ceramics and Materials Science
(617) 253-6835 01-4 $114,785

Fundamental study to characterize irradiation-induced amorphization of network silicas and pyrophosphates. Irradiations to be performed in-situ with electrons in a TEM, with heavy ions using the implantation facilities, or with neutrons using available neutron sources. Characterization by standard and energy-filtered electron diffraction techniques, high-resolution TEM imaging, Rutherford backscattering, high-performance liquid chromatography, IR spectroscopy, and differential scanning calorimetry. Various crystalling polymorphs of $SiO_2$, representing different combinatorial geometries in their network structures, vitreous silica, single crystals of $Pb_2P_2O_7$, and several phosphate glasses will be studied. A topological approach will be used in computer simulations to model both the structure and the amorphization.

**312. MICROSTRUCTURAL DESIGN IN CELLULAR MATERIALS**

L. J. Gibson, Department of Civil Engineering
(617) 253-7107 01-5 $83,074

Investigation of efficient microstructures for cellular solids through micromechanical modeling and production of cellular materials with the proposed microstructures. Characterization of the microstructure and mechanical properties of the materials. Comparison of the models with the experimental data. Comparison of the efficiencies of the proposed microstructures.

**313. SYSTEMATIC GLOBAL RENORMALIZATION-GROUP STUDIES OF DETAILED MODELS FOR CONDENSED MATTER SYSTEMS**

A. N. Berker, Department of Physics
(617) 253-2176 02-3 $44,065

Theoretical studies directed toward the eventual establishment of the position-space renormalization-group method (RGM) as a routine tool for use in condensed matter physics, with attempts to eliminate the ad hoc nature of the usual approximations used in the RGM. Improvement of the convergence, accuracy, and computational burden of the RGM by use of transformations, obtained with Monte Carlo sampling, to build in global phase diagram considerations. Extension of the RGM to treat rescaling behavior of quantum and continuum systems. Use of the new RGM techniques to treat novel physical phenomena such as the antiferromagnetic Potts model, the phase diagrams of selenium on Ni(100) and krypton on graphite, the chaotic rescaling of spin-glasses, and the hybrid-order phase transition of the random-field Ising model.

**314. CONSTRUCTION OF A SMALL ANGLE NEUTRON SCATTERING SPECTROMETER FOR INVESTIGATION OF MICROEMULSIONS AND MICELLAR SOLUTIONS IN BULK, IN POROUS MATERIALS AND UNDER SHEAR**

S.-H. Chen, Department of Nuclear Engineering
(617) 253-3810 03-2 $93,500

A special purpose small angle neutron scattering diffractometer at the Intense Pulsed Neutron Source (IPNS) of Argonne National Laboratory will be constructed. The diffractometer will be fully available to general users and will be constructed by a cooperative effort between the principal investigator and the IPNS staff with financial assistance from Texaco. The principal investigator will focus on the use of the diffractometer for studies of problems in the area of microemulsions and micellar solutions. For these investigations it is proposed to build a temperature controlled environment for scattering experiments and to build a shear cell for the study of shear fields on microemulsion and micelle structures.

## MIAMI (OHIO) UNIVERSITY
**Oxford, OH 45056**

**315. MAGNETIC MULTILAYER INTERFACE ANISOTROPY**
M. J. Pechan, Department of Physics
(513) 529-4518 02-2 $39,000

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

## MICHIGAN STATE UNIVERSITY
**East Lansing, MI 48824**

**316. HIGH TEMPERATURE STABILITY, INTERFACE BONDING, AND MECHANICAL BEHAVIOR IN B-NIAL AND NI3AL MATRIX COMPOSITES WITH REINFORCEMENTS MODIFIED BY ION BEAM ENHANCED DEPOSITION**
D. S. Grummon, Department of Metallurgy, Mechanics, and Materials Science
(517) 355-5141 01-2 $61,600

The microstructural stability and mechanical properties of reinforced ordered intermetallics(primarily -NiAl) by $Al_2O_3$ and SiC, particles, whiskers, and short fibers is investigated. Interfacial bonding is modified by an alumina coatings applied by ion beam enhanced deposition. High-temperature strength and low-temperature toughness will be measured.

**317. THEORETICAL STUDIES OF BREAKDOWN IN RANDOM MEDIA**
P. M. Duxbury, Department of Phyics and Astronomy
(517) 353-9179 01-3 $76,320

Scaling theories and numerical algorithms for predicting structure/extreme property relationships in random media. Use of concepts in statistical mechanics, disordered systems and nonequilibrium growth in conjuction with fracture mechanics, damage mechanics and dielectric breakdown to develop unified perspective of breakdown phenomena. Development of generic models and general methodology, and treatment of specific breakdown problems.

## MICHIGAN TECHNOLOGICAL UNIVERSITY
**Houghton, MI 49931**

**318. EFFECTS OF GRADIENTS ON BOUNDARY STABILITY**
S. Hackney, Department of Metallurgical Engineering
(906) 487-2170 01-1 $86,786

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

## UNIVERSITY OF MICHIGAN
**475 E. Jefferson**
**Ann Arbor, MI 48109-2136**

**319. FUNDAMENTAL ALLOY DESIGN OF OXIDE CERAMICS AND THEIR COMPOSITES**
I-W. Chen, Department of Materials Science and Engineering
(313) 763-4970 01-2 $84,165

Three alloy design approaches to oxide ceramics for structural and energy applications. Allovalent ions in solid solutions investigated for space charge segregation and effects on grain growth, dislocation creep and intergranular cavitation. Precipitation of spinel-based layers compounds studied for toughened and strengthened composites. Ceramic matrix composites with interpenetrating ductile phase prepared by infiltration of porous ceramic preforms with liquid under pressure. Structure property relationships established through variation of microchemical, microstructural, crystallographic and other material parameters.

**320. THE ROLE OF GRAIN BOUNDARY CHARACTER IN THE ENVIRONMENTALLY-ASSISTED INTERGRANULAR CRACKING MECHANISM OF NICKEL-BASE ALLOYS**
G. S. Was, Department of Nuclear Engineering
(313) 763-4675 01-2 $118,623

The objective of this program is to determine the role of the chemistry and structure of grain boundaries in the environmentally-assisted intergranular cracking (EAIC) of nickel-base alloys so that intergranular (IG) cracking can be ameliorated through control of grain boundary chemistry and structure. The focus is on the role of carbon in solution and as carbides on the IG creep-controlled cracking in 360C water; determination of the role of grain boundary orientation on IG cracking in 360C water and creep in 360C Ar; and the role of the film character (composition and structure) in the correlation of creep, repassivation rate, and IGSCC susceptibility in Ni-(16-30)Cr-Fe alloys. Experiments conducted on laboratory and commercial heats of Ni-16Cr-9Fe (alloy 600), Ni-30Cr-9Fe (alloy 690), and Ni-16Cr-9Fe-Al-Ti-Nb (alloy X-750).

**321. THE STRUCTURAL BASIS FOR FATIGUE INITIATION IN GLASSY POLYMERS**

A. F. Yee, Department of Materials Science and Engineering
(313) 764-4312 01-2 $93,086

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

**322. A FREE ENERGY SIMULATION METHOD BASED STUDY OF INTERFACIAL SEGREGATION**

D. J. Srolovitz, Department of Materials Science and Engineering
(313) 936-1740 01-3 $112,799

Theoretical methods and computer simulations to investigate the effects of segregation on the thermodynamic properties of grain boundaries and other interfaces in alloys. Application of a free energy simulation method to investigate the systematics of segregation at interfaces.

**323. SYNCHROTRON STUDIES OF NARROW BAND MATERIALS**

J. W. Allen, Department of Physics
(313) 763-1150 02-2 $50,000 (6 months)

Conduct a program of spectroscopic studies of the electronic structure of narrow band actinide, rare earth and transition metal materials, with emphasis on the use of synchrotron radiation as well as related laboratory spectroscopy. The spectroscopy will be directed toward aspects of the electronic structure which underlie or are responsible for novel ground state phenomena occurring in mixed valent, heavy-Fermion and high temperature superconductivity materials, including metal-insulator transitions. Data to be analyzed using density-functional calculations and many-body Hamiltonian models.

**324. GROWTH AND NONLINEARITY**

L. M. Sander, Department of Physics
(313) 764-4471

R. Savit, Department of Physics
(313) 764-3426 02-3 $150,000

Theoretical approach to gain an understanding of the relationships between growth mechanisms, structure, and properties of nonequilibrium systems, such as smoke, colloids, deposition of vapors and electrolytes which have been shown to give rise to scale invariant fractal-like structures. Objects of this type have a morphology which lies between conventionally studied crystalline geometry and the amorphous state. The unique properties of this kind of matter can be traced to the fact that it possesses an invariance property not shared by either crystalline or amorphous matter; that of non-trivial scale invariance. That is, the systems "look" the same on all length scales and scale with a generally non-integer dimension. The behavior of various kinds of random walks on these fractal clusters as well as the behavior of equilibrium statistical spin systems defined on the clusters will be of interest for understanding the dynamics of such random scale-invariant objects.

## UNIVERSITY OF MINNESOTA
**Minneapolis, MN 55455**

**325. CRYSTALLINE-AMORPHOUS INTERFACES AND AMORPHOUS FILMS IN GRAIN BOUNDARIES**

C.B. Carter, Department of Chemical Engineering and Materials Science
(607) 255-4797 01-1 $121,221

TEM investigation of structure and chemical composition of grain boundaries; kinetics of glass formation, thermodynamic equilibria; high-angle grain boundaries in MgO, twist boundaries and asymmetric tilt boundaries in Si and Ge, and low-angle grain boundaries in $Al_2O_2$; comparison of bicrystal samples with and without amorphous intergranular layer. Bicrystals formed by hot-pressing together two single crystals with or without an amorphous layer; thin foils reacted with $SiO_2$ vapor for investigations of grooving, film penetration and dewetting.

**326. MICROMECHANICS OF BRITTLE FRACTURE: STM, TEM, AND ELECTRON CHANNELING ANALYSIS**

W. W. Gerberich, Department of Chemical Engineering and Materials Science
(612) 625-8548 01-2 $87,496

Research to address (1) crack dynamics and inherent plasticity effects, (2) ligament contributions to fracture resistance and (3) micro-mechanics of final instability. Polycrystalline and single crystal materials investigated as a function of temperature, grain size and material thickness. Materials: Fe-3wt%Si single crystals, Au and Ir. Techniques include detailed fractography, acoustic emission, selected area channeling pattern (SACP) evaluation, cleavage modeling, TEM, impact and mechanical studies, AES, XPS, SIMS, UPS, EELS, and STM.

**327. FUNDAMENTAL STUDIES OF STRESS DISTRIBUTIONS AND STRESS RELAXATION IN OXIDE SCALES ON HIGH TEMPERATURE ALLOYS**

D. A. Shores, Department of Chemical Engineering and Materials Science
(612) 625-0014 01-3 $153,058

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

**328. MODELING AND EXPERIMENTAL STUDIES OF OXIDE COVERED METAL SURFACES**

W. H. Smyrl, Department of Chemical Engineering and Materials Science
(612) 625-0717 01-3 $141,044

Studies intended to characterize the ordered growth of oxide on titanium. Influence of growth conditions on the structure and texture of oxide films. Reflection, transmission, and scanning electron microscopy will be used. Local electron properties of oxide films investigated by photoelectrochemical microscopy. Calculation of the electron structure of various defects in thin films of titanium oxide. Vibrational Raman spectroscopy used as a diagnostic probe of the growth and structure of titanium oxide thin films. Determination of the growth and structure of titanium oxide thin films. Determination of the concentration and identity of structural defects in the oxide lattice.

**329. THEORY OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF SOLID STATE OXIDES**

J. R. Chelikowsky, Department of Chemical Engineering and Materials Science
(612) 625-4837 02-2 $60,000

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

## UNIVERSITY OF MISSOURI AT COLUMBIA
**Columbia, MO 65211**

**330. HIGH PRESSURE OPTICAL STUDIES OF SEMICONDUCTORS AND HETEROSTRUCTURES**

H. R. Chandrasekhar, Department of Physics and Astronomy
(314) 882-6086 02-2 $50,000

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

**331. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION**

W. B. Yelon, Department of Physics
(314) 882-5236 02-2 $50,000

This project aims at the development and use of ultra high intensity Mossbauer sources for scattering experiments. The technique has been shown to be feasible and it has been applied to the investigation of the precise character of the resonance line shape, anharmonicity in sodium, diffusive properties of organic liquids, and critical phenomena in charge density wave layer compounds.. Studies have been initiated in soft modes, phasons and interference with potential applications in testing possible violation of time reversal invariance in the electromagnetic decay of nuclei. The work is being carried out at the University of Missouri Research Reactor Facility and with a specially constructured scattering facility at Purdue University. Both conventional and conversion electron scattering techniques are being used, particularly microfoil conversion electron (MICE) detectors to enhance signal-to-off-resonance counting rates. This is a tightly coupled effort between Dr. Yelon and Professor Mullen at Purdue University.

## UNIVERSITY OF MISSOURI AT KANSAS CITY

**Kansas City, MO 64110-2499**

**332. THEORETICAL STUDIES ON THE ELECTRONICS STRUCTURE AND PROPERTIES OF CERAMIC CRYSTALS AND GLASSES**

W-Y. Ching, Department of Physics
(816) 235-2503 01-1 $127,903

Calculation by means of orthogonalized linear combination of atomic obitals (OLCAO) local density functional of electronic structure and linear optical properties for a larger number of oxide, nitride, phosphate, silicate, III-V semiconductors, metallic glass and high $T_c$ superconducting materials approximation. Calculation of important bulk properties, phonon frequencies and structural phase transitions for selected materials. Formulation of calculational method for nonlinear optical properties. Calculation of magnetic properties of rare earth-iron-boron magnetic alloys and related intermetallic compounds.

## UNIVERSITY OF MISSOURI AT ROLLA

**278 McNutt Hall**
**Rolla, MO 65401**

**333. CHARACTERIZATION OF ELECTICALLY CONDUCTING OXIDES**

H. U. Anderson, Department of Ceramic Engineering
(314) 341-4886 01-3 $116,000

Interrelationships between electrical conductivity, oxidation reduction kinetics, defect structure, and composition for transition metal perovskites based on Cr, Mn, Fe and Co. Focus on role of transition metal ions and other crystallographic and thermodynamic factors that control the relative amounts of mixed ionic/electronic conductivity. Experimental techniques include specimen preparation, thermogravimetric characterization, optical microscopy, X-ray and neutron diffraction, TEM, electrical conductivity, Seebeck coefficient studies, thermal and optical stimulated current spectroscopy and deep level transient spectroscopy.

## MONTANA STATE UNIVERSITY

**Bozeman, MT 59717**

**334. ELECTROACTIVE POLYMERS AND LIQUID CRYSTALS**

V. H. Schmidt, Department of Physics
(406) 994-6173 03-2 $47,000

Study of chain conformation, rotations, and other motions in the piezoelectric polymers, polyvinylidene fluoride, and its copolymer with trifluoroethylene by NMR and optical techniques. Pressure and temperature dependence on the nonferroelectric to ferroelectric phase transitions. NMR of deuterated samples and optical studies involving birefringence, small angle light scattering, and Brillouin scattering to measure degree of chain alignment and sound velocity and attenuation as affected by polymer processing and by temperature and pressure induced phase transitions including theoretical studies of crystal elastic energy and statistical mechanics of linear polymers.

## NATIONAL ACADEMY OF SCIENCES

**2101 Constitution Avenue**
**Washington, D.C. 20418**

**335. POLYMER SCIENCE AND ENGINEERING: THE SHIFTING RESEARCH FRONTIER**

D. J. Raber, Department of Chemical Sciences and Technology
(202) 334-2156 03-1 $20,000

Support for an assessment of the state of polymer sciences and engineering to identify research opportunities and needs and to provide prioritization of these opportunities.

**336. AN ASSESSMENT OF NEUTRON-SCATTERING SCIENCE**

D. C. Shapero, Department of Physics and Astronomy
(202) 334-3520 03-1 $145,000

Support for an assessment of the state of neutron-scattering science and to identify research opportunities. Emphasis will be placed on optimization of instrumentation for the scientific use of the ANS.

## UNIVERSITY OF NEBRASKA
**Lincoln, NE 68588-0113**

**337. FUNDAMENTAL STUDIES OF STRONGLY MAGNETIC RARE EARTH-TRANSITION METAL ALLOYS**
D. J. Sellmyer, Department of Physics
(402) 472-2407 02-2 $75,000

Research to advance the understanding of new, strongly magnetic rare earth-transition metal compounds and alloys. Magnetic phases studied are based on iron and light rare earths, and are generally ternary or higher order alloys with unusually complex, anisotropic structures. The type of systems investigated include new Fe-rich phases which are nitrogenated or carbonated to enhance their magnetic properties, new phases reached by intermediate metastable phases via melt spinning, and sputtered thin films and multilayers. Comprehensive experiments performed include X-ray and neutron diffraction, electron microscopy, dc and ac magnetic susceptibilities, Mossbauer spectroscopy, and photoemission. Experimental results compared with spin-polarized, self-consistent electronic structure calculations. Research performed in close collaboration with work at the University of Delaware.

## UNIVERSITY OF NEVADA
**Reno, NV 89557**

**338. PHOTOPHYSICAL PROPERTIES OF TRIPLET EXCITATIONS ON POLYMERIC SYSTEMS**
R. D. Burkhart, Department of Chemistry
(702) 784-6041 03-1 $106,250 (15 months)

Studies of triplet-triplet annihilation and rate of triplet exciton diffusion in polymers. Studies of delayed luminescence processes in organic polymers to determine the extend and influence of recombination of geminate ion pairs. Direct excitation of ground state polymer chromophores to lowest triplet state through dye laser pumping. Investigation of the rate of triplet exciton migration in polymers having pendant groups which are sterically crowded and non-planar to assess the extent to which structural modifications can influence rates of exciton migration. Modification of the rate of triplet-triplet annihilation by microwave-induced mixing, monitor the dependence of triplet quantum yields on the energy of excitation, and to probe the direct detection of carbazole radical cations by transient absorption spectroscopy.

## UNIVERSITY OF NEW HAMPSHIRE
**Durham, NH 03824**

**339. EFFECTS OF FRACTURE SURFACE INTERFERENCE ON SHEAR CRACK GROWTH**
T. S. Gross, Department of Mechanical Engineering
(603) 862-1352 01-2 $86,481 (10 months)

An experimental and theoretical program to study the effects of fracture surface interference on shear modes (mode II and III) of crack growth. The theoretical program to extend and refine current models of force transfer between crack faces and wear of asperities in the vicinity of the crack tip. The model will be the observed non-monotonic, non-linear dependence of shear crack growth on applied shear stress, superimposed tensile stress, and cyclic load history. The experimental program to study the evolution of fracture surface roughness using Fourier analysis to characterize the average asperity amplitude, slope, and wavelength of fracture surface profiles in a variety of loading configurations and environmental conditions for metals, ceramics, and polymers. A broad range of materials selected for testing to maximize the variation in elastic modulus, yield strength, fracture surface profile and wear characteristics.

## UNIVERSITY OF NEW MEXICO
**Albuquerque, NM 87131**

**340. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE SILICATES, COMPLEX OXIDES, AND PHOSPHATES**
R. C. Ewing, Department of Geology
(505) 277-4163 01-1 $113,082

Investigation of radiation effects in naturally-damaged minerals and ion-implanted ceramics. Emphasis on reaction paths to aperiodic state, microstructure and bonding in fully damaged materials, annealing kinetics and mechanisms, and recrystallization/alteration products. Techniques include X-ray diffraction, high-resolution transmission electron microscopy (HRTEM), extended X-ray absorption fine-structure spectroscopy (EXAFS), and near-edge spectroscopy (XANDES). Materials studied include zircon ($ZrSiSiO_4$), thorite/huttonite ($ThSiO_4$), monazite ($CePO_4$), titanite ($CaTiSiO_5$), and uraninite ($UO_2$).

**341. ADSORPTION STUDIES AT A SOLID-LIQUID INTERFACE**
J. A. Panitz, Deparment of Physics
(505) 277-8488 01-1 $147,408

Adsorption phenomena at a solid-liquid interface. Monolayer films and multilayer structures formed on metal and semiconductor surfaces by Langmuir-Blodgett and simple diffusive adsorption from aqueous solution. Surface morphology, adsorbate conformation, and chemical analysis of interface mapped in high vacuum on a subnanometer scale using a new instrument that combines high-resolution transmission electron microscopy with imaging atom-probe mass spectroscopy. Vitreous ice, formed from the native environment, used to cryoprotect the interface, allowing the embedded interface and the species adsorbed on its surface to be transferred into high vacuum for analysis without modification or damage.

## NORTH CAROLINA STATE UNIVERSITY
**Raleigh, NC 27695**

**342. THE STUDY OF STRUCTURE-PROCESSING-PROPERTY RELATIONS IN COPPER OXIDE-BASED HIGH TC SUPERCONDUCTORS**
A. I. Kingon, Department of Materials Science and Engineering
(919) 515-2377 01-1 $108,798

Relationships between the crystallographic and electronic structure of copper oxide-based compounds and their electronic and superconducting properties. Study of aspects controlling grain boundary composition and growth to provide structure-properties relationship. Measurement of transport $J_c$ across isolated grain boundaries.

**343. CRACK GROWTH RESISTANCE BEHAVIOR IN TOUGHENED CERAMICS**
R. O. Scattergood, Department of Materials Science and Engineering
(919) 515-7843 01-5 $101,836

Systematic study of fundamental aspects of erosion and impact damage in brittle materials and advanced ceramic systems. Materials investigated include aluminas, fiber-reinforced ceramics, transformation-toughened ceramics and various model brittle materials. New or modified apparatus designed and constructed for particle properties and threshold effects. Experimental results on erosion behavior and impact damage utilized for new fracture-mechanics analyses and erosion models development. Erosion rates vs. particle sizes, velocities and impact angles. Characterization of microstructural, strength and fracture properties. Erodent particle properties influence on nature of threshold effects.

**344. RESEARCH AT AND OPERATION OF THE MATERIAL SCIENCE X-RAY ABSORPTION BEAMLINE (X-11) AT THE NATIONAL SYNCHROTRON LIGHT SOURCE**
D. E. Sayers, Department of Physics
(919) 737-2512 02-2 $280,000

Development, improvement, and operation of beamlines X-11A and B at the National Synchrotron Light Source, Brookhaven National Laboratory. Transmission, fluorescence electron-yield and X-ray absorption fine structure measurements on a range of materials and interfaces, including metal-semiconductor systems; multilayers and ion implanted layers; electrochemical systems; rare earth metal oxide catalysts; semiconductor alloys; high-$T_c$ superconductors; biocatalysts and actinide metals.

**345. BAND ELECTRONIC STRUCTURES AND CRYSTAL PACKING FORCES**
M. H. Whangbo, Department of Chemistry
(919) 515-3464 03-1 $125,000

Theoretical investigation of the electronic and structural properties of various low-dimensional solid state materials, which include: (1) organic conducting and fullerene salts, (2) cuprate superconductors, and (3) transition-metal compounds. The primary techniques for the investigation are tight-binding electronic structure calculations and ab initio self-consistent-field/molecular-orbital (SCF-MO) approaches. The main objectives of the project are to search for structure-property correlations which serve to govern the physical properties of the various materials, and to develop a library of efficient computer programs for the calculation of the physical properties of low-dimensional solid state materials.

**346. THEORETICAL STUDIES OF SURFACE REACTION ON METALS AND ELECTRONIC MATERIALS**
J. L. Whitten, Department of Chemistry
(919) 737-7277 03-1 $83,000

Theoretical studies of the adsorption of small molecules and molecular fragments on the surfaces of nickel and silicon using the embedding formulation of ad initio calculations. Energy contours and preferred surface adsorption sites are calculated along with vibrational frequencies for adsorbates. In some cases, excited electronic states will be calculated to help sort out the direct ionization vs. Auger processes that relate to electron or photon stimulated desorption from silicon surfaces. The embedding scheme is uniquely suited to these computations.

## NORTHEASTERN UNIVERSITY
**360 Huntington Avenue**
**Boston, MA 02115**

**347. COMPUTER MODELING OF SOLIDIFICATION MICROSTRUCTURE**
A.S. Karma, Department of Physics
(617) 437-2929 01-5 $63,698

The irregular structures formed in Fe-C and Al-Si irregular eutectic alloys have remained poorly understood in comparison to the regular lamellar and rod-like morphologies which form in metal-metal eutectic alloys. Banding is a novel microstructure widely observed in rapidly solidified metallic alloys which is characterized by structural variations in time so as to produce alternating bands parallel to the solidification front. Numerical models will be developed to cope with both irregular eutectic and banded microstructures, and make specific predictions which can be tested against existing experimental data.

## NORTHWESTERN UNIVERSITY
**Evanston, IL 60208**

**348. ATOMIC RESOLUTION ANALYTICAL ELECTRON MICROSCOPY OF GRAIN BOUNDARY PHENOMENA ASSOCIATED WITH ISOLATED-SINGLE GRAIN BOUNDARIES IN BICRYSTALS OF SRTIO3**
V.P. Dravid, Department of Materials Science and Engineering
(708) 467-1363 01-1 $133,000 (20 months)

Grain boundary atomic structure, bicrystallography, local chemistry, dielectric function, and electronic structure determined for isolated individual grain boundaries in oriented bicrystals of $SrTiO_3$-based varistors and grain boundary layer capacitors; bicrystals of predefined angular misorientation and interface plane, with and without dopants, and under various appropriate heat treatment conditions. Cold-field emission TEM-atomic resolution analytical electron microscopy (ARAEM), ultrahigh vacuum HREM under ultraclean conditions; electronic structure and local dielectric function of the grain boundary region using EELS fine structure analysis; I-V curve and complex impedance analysis of the bicrystals as function of grain boundary parameters.

**349. DEFECT CLUSTERING IN SIMPLE AND COMPLEX OXIDES**
T. O. Mason, Department of Materials Science and Engineering
(708) 491-3198

D. E. Ellis, Department of Physics and Astronomy
(708) 491-3665 01-1 $176,967

Study of defect clustering and related properties of oxides involving transport and nonstoichiometry measurements, diffraction, microscopy, and quantum theoretical methods. Oxides of interest include highly defective transition metal monoxides (Fe, MnO, CoO, NiO), transition metal spinels ($Fe_3O_4$ and $Mn_3O_4$), stabilized $ZrO_2$, and ternary systems, such as $CaxNi_{1-x}O$ and high-$T_c$ superconductors. Transport and nonstoichiometry studies in a high oxygen potential cell that permits substantially higher defect concentrations to be achieved. Structural and valence studies by X-ray and neutron diffraction, electron microscopy, and near-edge absorption spectroscopy. Finite temperature modeling (using molecular dynamic and statistical mechanics approaches) of defects in monoxides and total energy calculations of defect arrangements in complex oxides. Modeling of defect dependent properties of materials.

**350. ATOMIC STRUCTURES AND COMPOSITIONS OF INTERNAL INTERFACES**
D. N. Seidman, Department of Materials Science and Engineering
(708) 491-4391 01-1 $99,833

Fundamental relationships between structures and chemical compositions of metal/ceramic heterophase interfaces. Transmission electron microscopy, high resolution electron microscopy, analytical electron microscopy and atom-probe field-ion microscopy are utilized to study the structure and chemistry of metal/ceramic interfaces. The use of ternary alloys allows for the possibility of studying solute-atom segregation effects at heterophase interfaces; this is an area where very little information exists. Trapping of hydrogen at heterophase interfaces is studied via atom probe microscopy. Some of the systems being studied are: Cu/MgO, $Ni/Cr_2O_3$, Cu/BeO, Cu/NiO, Cu/Mg, $Ta(W)/HfO_2$, $Fe(Sn)/Al_2O_3$, $Fe(P)/Al_2O_3$, $Fe(Ni)/Al_2O_3$, $NiO/NiCr_2O_4$, $Ni(Al)/NiAl_2O_4$, Ph(H)/MgO and Cu(H)/MgO. The atom probe measurements, in conjunction with different electron microscopies, yield unique atomic scale information about these heterophase interfaces.

**351. TRANSFORMATION PLASTICITY IN DUCTILE SOLIDS**
G. B. Olson, Department of Materials Science and Engineering
(708) 491-2847 01-2 $138,829

Mechanisms of transformation toughening in ductile solids investigated by (a) detailed observations of crack-tip processes, and (b) numerical modeling with experimentally-derived constitutive relations. Model alloy steels ($\gamma$-strengthened and phosphocarbide strengthened steels) used to study room temperature transformation toughening and constitutive behavior. Shear-instability-controlled fracture observed at sectional crack tips with and without transformation plasticity interactions using alloy composition to vary phase stability. Quantitative constitutive relation for experimental alloys applied to crack-tip and notch fields to study transformation plasticity interaction with various models of microvoid-softening-induced shear localization.

**352. STUDY OF MECHANICAL BEHAVIOR AND INTERNAL STRUCTURE OF FERRITIC NANOCRYSTALLINE MATERIAL**
J. R. Weertman, Department of Materials Science and Engineering
(708) 491-3537 01-2 $106,602

Investigation of the fundamentals of mechanical behavior of nanocrystalline iron and steel. The influence of decreasing grain size and interstitial content on the tensile and creep strength will be examined in nanocrystalline iron made by the inert gas condensation method. Some samples will be carburized or nitrided before testing. Small angle scattering (both X-ray and neutron), high-resolution electron microscopy and analytical electron microscopy, precision density measurements, and X-ray diffraction will be used to obtain detailed information about the internal structure of the material. This information will be used as a guide to interpreting results of the mechanical measurements.

**353. PLASMA, PHOTON, AND BEAM SYNTHESIS OF DIAMOND FILMS AND MULTILAYERED STRUCTURES**
R. P. H. Chang, Department of Materials Science and Engineering
(708) 491-3598 01-3 $73,753

Deposition of polycrystalline diamond films with hydrogen plasma; effects of process conditions, including gas pressure, charged species in plasma, metallic and ceramic substrates, surface chemistry, role of interfacial layer in promoting adhesion; film structure, graphite inclusion. Investigation of gas phase nucleation of diamond particles.

**354. DEFECT STRUCTURE OF SEMICONDUCTING AND EPITAXIAL INSULATING OXIDES**
B. W. Wessels, Department of Materials Sciences and Engineering
(312) 491-3219 01-3 $70,381

Defect pheonomena in oxides including electrical activity of native defect states, charge compensation mechanisms in deliberately doped material, transition and rare-earth metal related defects, and electronic states associated with extended defects. Preparation of perovskite-type thin film oxides, including $SrTiO_3$, $BaTiO_3$, $(BaSr)TiO_3$ and $Bi_4Ti_3O_{12}$, by organometallic chemical vapor deposition. Defect structure analyzed by deep level transient spectroscopy, deep level optical spectroscopy, photoluminescnece, Hall effect measurements and transmission electron microscopy; optical and electronic properties and thermal stability of defects determined.

**355. DEPOSITION AND PROPERTIES OF NOVEL NITRIDE SUPERLATTICE COATINGS**
S. A. Barnett, Department of Materials Science and Engineering
(708) 491-2447

W. D. Sproul, Department of Materials Science and Engineering
(708) 491-4108 01-5 $76,982 (10 months)

Deposition and properties of nitride-nitride superlattices, TiN/VN and TiN/NbN, and nitride superlattices contained in metal layers, TiN/Ni and TiN/NiCr, on steel substrates. High-rate reactive deposition by magnetron sputtering; characterization of lattice constants and superlattice constants, microstructure, microhardness, adhesion, stress, thermal expansion coefficient and film biaxial elastic modulus.

**356. ENERGETICS, BONDING MECHANISM AND ELECTRONIC STRUCTURE OF METAL/CERAMIC INTERFACES**
A. J. Freeman, Department of Physics and Astronomy
(708) 491-3343 02-3 $50,000 (5 months)

Model the energetics, bonding, bonding mechanism and structure of metal/ceramic interfaces. Investigate surface electronic structure of oxides and interface grain boundaries in transition metal-simple oxide interfaces, e.g., Pd- and Nb-alumina interfaces as well as metal/SiC interfaces. Investigations of ferroelectricity in lead titanate and antiferroelectricity in lead zirconate. Investigations of the electronic structure of $TiO_2$ surfaces and the properties and structures of $VO_2/TiO_2$ interface.

**357. MIXED IONIC AND ELECTRONIC CONDUCTIVITY IN POLYMERS**

M. A. Ratner, Department of Chemistry
(708) 491-5652

D. F. Shriver, Department of Physics
(708) 491-5655 03-2 $94,000

Investigation of ionic transport along and through interfaces, both within a given solid electrode or electrolyte and between solid electrodes and electrolytes. The objective is mechanistic understanding of which processes result in overpotential, degradation, charge accumulation, and enhanced mobility at such interfaces. Two general classes of materials will be investigated: siloxane based polymer electrolytes, and layered chalcogenide cathodes. Experiments will include synthesis and surface modification of electrolyte films, bulk and interfacial impedance measurements, and simulation of interfacial transport phenomena by Monte Carlo and percolation theory techniques.

**358. STRUCTURE SHEAR RESPONSE AND TRANSFER PROPERTIES OF LIPID MONOLAYERS**

P. Dutta, Department of Physics
(708) 491-5465

J. B. Ketterson, Department of Physics
(708) 491-5468 03-3 $89,354

Study the mechanical properties of organic monolayers on the surface of water (Langmuir films). Determine the microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) using ellipsometry, conventional and synchrotron X-rays. Mechanical property studies directed toward shear response, and important but previously neglected structural property. Diffraction technique, involving external reflection at the monolayer surface, used to determine film structure. Use standing-wave fluorscence technique to determine the distribution of ions in the aqueous phase near the head groups in lipid monolayer films.

## UNIVERSITY OF NOTRE DAME
**Notre Dame, IN 46556**

**359. SINGLE-ELECTRON TUNNELING**

S. T. Ruggiero, Department of Physics
(219) 239-7463 02-2 $49,000

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

## OHIO STATE UNIVERSITY
**Columbus, OH 43210**

**360. EFFECT OF ALLOYING ELEMENTS ON PASSIVITY AND BREAKDOWN OF PASSIVITY OF FE- AND NI-BASED ALLOYS. MECHANISTICS ASPECTS**

Z Szklarska-Smialowska, Department of Materials Engineering
(614) 292-0290 01-5 $65,000

Mechanism of pitting corrosion of Al-alloys. Pit development and solubility of oxidized alloying elements in acid solutions. Susceptibility to pitting in the composition of oxide films. Fe- and Ni- alloys produced by sputtering deposition method.

**361. THEORY OF EXOTIC SUPERCONDUCTING AND NORMAL STATES OF HEAVY ELECTRON AND HIGH TC MATERIALS**

D. Cox, Department of Physics
(614) 292-0620 02-3 $34,000 (8 months)

Quadropole fluctuation mediated superconductivity in heavy electron systems. Investigation of the effect of quadrupolar fluctuations on the superconductivity of $UBe_{13}$. Application of self consistent conserving approximations to Anderson Lattice Models of heavy electron systems. Exploration of quadrupolar fluctuation induced superconductivity in the four band Anderson Lattice Model.

**362. STRONGLY INTERACTING FERMION SYSTEMS**

J. W. Wilkins, Department of Physics
(614) 292-5193 02-3 $130,000

Development of new methods for calculating electronic properties, specifically, electronic structure, and the physics of materials associated with high temperature superconductors. Algorithm development to include new schemes for constructing Wannier functions and applying Quantum Monte Carlo techniques for studying the ground state and low temperature properties of important highly correlated systems. Local equilibrium atomic geometry in very thin semiconductor superlattices and the development of methods for understanding the forces that determine stability and instability. Adatom induced reconstruction of transition metals. Application of a modified Hubbard model to high-$T_c$ superconductors to explain the role of the oxygen hole; application of a Quantum Monte Carlo code for the Anderson Lattice to determine the possibility of antiferromagnetism and superconductivity in these materials.

## OHIO UNIVERSITY
**Athens, OH 45701**

### 363. ELECTRONIC STATES IN SYSTEMS OF REDUCED DIMENSIONALITY
S. E. Ulloa, Department of Physics and Astronomy
(614) 593-1729 02-3 $50,000

Theory of semiconductor systems, specifically those where electrons are confined to regions of only a few Fermi wavelengths. Work includes the effects of geometrical confinement and its interrelationship with electric and magnetic fields and transport properties of systems in the ballistic and near-ballistic regimes. Confined systems will be investigated to determine whether confinement induces collective and single-particle modes in their optical response. Transport issues to be investigated will include the loss of phase coherence by elastic and inelastic scattering, transit times and the character of the tunneling mechanism.

## OKLAHOMA STATE UNIVERSITY
**Stillwater, OK 74078**

### 364. RHEO-OPTICAL STUDIES OF MODEL "HARD SPHERE" SUSPENSIONS
B. J. Ackerson, Department of Physics
(405) 744-5819 01-3 $75,181

Spontaneous and artifically induced microstructure of particles in suspensions of hard spheres; effect of microstructure on macroscopic properties. Interparticle order induced by shear flows and rheological properties; use of velocimetry techniques to determine microscopic flow properties; microstructure induced by sedimentation with and without shear; growth rate of hard sphere crystals.

## OREGON STATE UNIVERSITY
**Corvallis, OR 97331**

### 365. HYPERFINE EXPERIMENTAL INVESTIGATION OF ZIRCONIA CERAMICS
J. A. Gardner, Department of Physics
(503) 737-3278 01-1 $108,892

Perturbed angular correlation (PAC) spectroscopy of nuclear gamma rays to investigate Zr-containing ceramics. PAC characterization of free energies, transformation mechanisms, equilibrium phase boundaries, diffusion and relaxation models, short range order, order-disorder reactions, and elevated-temperature/time dependent effects in various zirconia-based ceramics that contain either Hf-181 or In-111 as a probe. Investigation of Zr-91 in zirconia by nuclear quadrupole resonance (NQR) and of 0-17 substituted zirconia by nuclear magnetic resonance (NMR). NQR/NMR experiments to complement and expand the studies of local structure and oxygen vacancy dynamics underway with PAC.

### 366. THEORETICAL STUDIES OF ZIRCONIA AND RELATED MATERIALS
H. J. F. Jansen, Department of Physics
(503) 737-1690 01-3 $76,304

Total energy calculations of the electronic structure of zirconia and related materials used to obtain the electronic energy and the charge density as a function of atomic arrangement. Study of field-gradients, lattice relaxation, phonon spectrum, oxygen mobility and transport. Both Full Potential Linearized Augmented Plane Wave (FLAPW), Monte Carlo and molecular dynamics techniques used.

## UNIVERSITY OF OREGON
**Eugene, OR 97403-0237**

### 367. SURFACE AND INTERFACE ELECTRONIC STRUCTURE
S. D. Kevan, Department of Physics
(503) 346-4742 02-2 $126,000

Experimental characterization of the electronic structure of clean and adsorbate-covered metal surfaces using high resolution angle resolved photoemission spectroscopy at the National Synchrotron Light Source. Emphasis is on relativistic effects on surface electronic and geometric structures, determination of Fermi surfaces for surface localized states, and characterization of resonant electronic states. Metals to be investigated include the 4d and 5d transition metals.

**368. MONITORING INTERFACIAL DYNAMICS BY PULSED LASER TECHNIQUES**
G. L. Richmond, Department of Chemistry
(503) 346-4635 03-2 $122,500 (15 months)

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 to femtosecond timescale, correlation of surface structure with electron transfer kinetics, thin-film nucleation and growth, and analyses of the structure and reactive role of surface defects.

## PENNSYLVANIA STATE UNIVERSITY
**332 Davney Laboratory**
**University Park, PA 16802**

**369. VIBRATIONAL AND ELECTRONIC PROPERTIES OF CLUSTERS AND ULTRATHIN FILMS**
J. S. Lannin, Department of Physics
(814) 865-9231 01-1 $102,430

Study of clusters and cluster-assembled ultrathin films and interfaces. Measurements of the influence of deposition conditions, substrate system, influence of hydrogen on substrate and film properties and changes in film deposition conditions. Characterization techniques include Raman scattering, ultraviolet photoemission spectroscopy, Auger spectroscopy, fiber optic-based ellipsometry and transmission electron microscopy. Research on elemental semimetallic, metallic and semiconducting systems; elements include Sb, C, Sn and Bi.

**370. FRACTURE BEHAVIOR OF SURFACE MODIFIED CERAMICS**
D. J. Green, Materials Science and Engineering
(814) 863-2011 01-2 $70,400

Modification of surface layers of ceramics to introduce surface compression to increase hardness and fracture toughness. 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 profiles determined by strain gauge techniques.

**371. FUNDAMENTAL STUDIES OF PASSIVITY AND PASSIVITY BREAKDOWN**
D. D. MacDonald, Department of Materials Science and Engineering
(814) 863-7772 01-3 $158,692

Study of the effects of minor alloying elements on passivity breakdown and of photo effects on properties of passive films. Use of electrochemical and photoelectrochemical techniques to explore transport and kinetic properties of vacancies and charge carriers in films and at metal/film and film/solution interfaces. Development of point defect and solute/vacancy interaction models. Electrochemical impedance spectroscopy to determine transport properties of vacancies in passive films and to explore kinetics of vacancy generation and annihilation at metal/film and film/solution interfaces. Kinetics of localized attack. Design new corrosion-resistant alloys and explore susceptibilities of existing alloys to pitting corrosion.

**372. INFLUENCE OF POINT DEFECTS ON GRAIN BOUNDARY DIFFUSION IN OXIDES**
V. S. Stubican, Department of Ceramic Science and Engineering
(814) 865-9921 01-3 $61,600

Investigation of grain boundary diffusion in bicrystals of $Fe_{3-x}O$ and $Ni_{1-x}O$ as a function of temperature and oxygen partial pressure in intrinsic defect region. Boundary chemistry to be characterized by Auger spectroscopy and TEM. Results evaluated using defect chemistry and compared to volume diffusion.

**373. INTERFACIAL PHENOMENA IN LASER WELDING**
T. DebRoy, Materials Science and Engineering
(814) 865-1974 01-5 $100,015

Improved composition control and properties of weld metal through basic understanding of interfacial chemistry and control of interstitial impurities. Dissolution of nitrogen, oxygen and hydrogen in weld metal under simulated and actual welding conditions. Improved physical understanding of the dynamics of liquid metal ejection during laser welding. Incorporation of improved interfacial physics and chemistry in numerical simulation of weld pool mass transfer. Parameters affecting mass transfer. Ongoing collaborative program with Oak Ridge National Laboratory.

**374. MULTIFUNCTIONAL NANOCOMPOSITE MATERIALS**
R. Roy, Materials Research Laboratory
(814) 865-3421

S. Komarneni, Materials Research Laboratrory
(814) 865-1542 03-2 $66,300

Synthesis and characterization of crystalline materials formed at low temperatures by topotactic and epitactic routes. The objective is to apply some of the very new and exciting advances in chemically-bonded ceramics to making much stronger and more impermeable materials that can be processed at low temperatures. The material has potential application as low-level radioactive waste hosts.

## UNIVERSITY OF PENNSYLVANIA
**Philadelphia, PA 19104**

**375. ATOMIC BONDING AT CERAMIC INTERFACES USING SCANNING TUNNELING MICROSCOPY**
D. A. Bonnell, Department of Materials Science and Engineering
(215) 898-6231 01-1 $74,375

Investigation on the effects of interfacial chemistry on the bonding and electronic structure at ceramic interfaces using scanning tunneling microscopy (STM), tunneling spectroscopy (TS), and transmission electron microscopy (TEM). Develop improved understanding regarding the imaging of large band gap structures in STM. Studies to include ZnO/ZnO, ZnO/ crystalline second phase, ZnO/amorphous second phase, and Si/Si (as model material) interfaces.

**376. STRUCTURE AND DYNAMICS IN LOW-DIMENSIONAL GUEST-HOST SOLIDS**
J. E. Fischer, Deparment of Materials Science and Engineering
(215) 898-6924 01-1 $141,140

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

**377. ATOMISTIC STUDIES OF GRAIN BOUNDARIES IN ALLOYS AND COMPOUNDS**
V. Vitek, Department of Materials Science and Engineering
(215) 898-7883 01-1 $112,983

Atomistic computer simulation studies of grain boundaries in binary ordered and disordered alloys. Investigation of grain boundaries with segregated solutes. Examination of the relationship between grain boundary structure and surfaces formed by fracturing along these boundaries. Study of grain boundary electronic structure. Methods of calculation of interatomic forces. $Ni_3Al$, $Cu_3Au$, Cu Au and Ni Al are candidate alloys to be studied.

**378. THE ROLE OF SLIP GEOMETRY AND HARDENING BEHAVIOR IN INTERGRANULAR TOUGHNESS**
C. Laird, Department of Materials Science and Engineering
(215) 898-6664

J. L. Bassani, Department of Mechanical Engineering and Applied Mechanics
(215) 898-5632 01-2 $138,538

Study of micromechanics of deformation and fracture processes at grain boundaries as affected by the structure of the boundary, slip geometry, hardening under multiple slip deformation, and the incompatibility of deformation at the boundary. Monotonic and cyclic experiments will focus on copper bicrystals and slip line analysis. TEM will be combined with continuum methods. The behavior of copper will be compared to Cu-Al having different stacking fault energies and a planar-slip mode.

**379. CONDENSED MATTER PHYSICS AT SURFACES AND INTERFACES OF SOLIDS**
E. J. Mele, Department of Physics
(215) 898-3135 02-3 $55,500

Theoretical studies of the lattice dynamics of reconstructed semiconductor surfaces. Computations, employing a developed theoretical model, will be used to investigate the effects of surface defect configurations through the surface elastic properties, the effects of simple commensurate surface defects and the effects of defect configurations which break the translational symmetry parallel to the surface. The systems will be investigated by a generalization of a long wavelength elastic theory to describe scattering of elastic waves by the various surface and figurations. An investigation of the dynamics of strongly correlated many-Fermion systems near the Mott insulating limit will be made.

## UNIVERSITY OF PITTSBURGH
**Pittsburgh, PA 15261**

**380. THE RELATIONSHIP BETWEEN MICROSTRUCTURE AND MAGNETIC PROPERTIES IN HIGH-ENERGY PERMANENT MAGNETS CHARACTERIZED BY POLYTWINNED STRUCTURES**
W. A. Soffa, Department of Materials and Engineering
(412) 624-9728 01-3 $99,128

The fundamental basis for the enhanced coercivities exhibited by melt-spun equiatomic Fe-Pd alloys compared to the bulk are investigated. This includes quantitative work comparing the scale of the microtwins and APB in bulk alloys and melt-spun ribbon, and in-situ observations of domain wall motion investigated. An APB pinning model will be established, and the energetics of thermally activated wall motion will be addressed.

**381. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES**
J. V. Maher, Department of Physics and Astronomy
(412) 624-9007 02-2 $114,000

Study of both the formation of patterns at liquid interfaces and the behavior of interfaces inside disordered systems. One experiment will study pattern development in a Hele-Shaw cell which has a uniformly changing gap. A second experiment will examine the effect of etched-plate anisotropy on patterns in a Hele-Shaw cell under a variety of conditions, in all cases where the length scale of the etchings are very well controlled and much smaller than the smallest length scale in the pattern. Three other experiments will study the underlying physics which determines the lower-length-scale selection in three distinctly different conditions for patterns between miscible liquids. A final set of experiments will investigate the formation of adsorption/wetting layers on polystyrene spheres in very dilute colloidal suspensions of these spheres in binary liquid mixtures, under conditions where the liquid correlation length is comparable to the radius of the spheres.

**382. COMPUTER SIMULATIONS FOR THE ADSORPTION OF POLYMERS AND SURFACES**
A. C. Balazs, Department of Materials Science and Engineering
(412) 648-9250 03-2 $36,000

Computer simulations and theoretical models to examine how the self-association reactions of amphiphilic polymers affect surface adsorption. Of particular interest is understanding how the architecture of the polymer chain and conditions such as the nature of the surface or solvent affect the extent of adsorption and the morphology of the interfacial layers. By understanding the factors that affect adsorption, predictions of chain geometries and conditions will yield the optimal interfacial sturcture for such applications as steric stabilization, adhesion and film growth. The significant advantage of computer simulations is that currently they are the only "experimental" tool with which one can simultaneously visualize the geometry of these self-assembled chains in solution, the comformation of the chains adsorbed directly to the surface and the microstructure of the entire interfacial region.

## POLYTECHNIC UNIVERSITY
**Brooklyn, NY 11201**

**383. SCANNING TUNNELING MICROSPECTROSCOPY OF SOLIDS AND SURFACES**
E. Wolf, Department of Physics
(718) 260-3080 02-2 $96,000

Development of Scanning Tunneling Microscopy (STM) techniques as applied to the study of solids and surfaces. Probe both normal and superconducting states of materials. Basic information about the new class of many-body states in heavy Fermion materials. Pairing symmetry study of $La_{1.8}Sr_{0.2}CuO_4$ a new high temperature superconductor. Basic superconducting tunneling phenomena; Josephson and proximity effects. Importance of spin-orbit coupling arising from the f-electron character of the heavy quasiparticles in heavy Fermion materials. Quasiparticle spectroscopy of exotic conductors including organic superconductors.

**384. SHORT RANGE ORDER EFFECTS: CERIUM AND ACTINIDE MATERIALS**
P. Riseborough, Department of Physics
(718) 260-3675 02-3 $56,695

Theoretical studies of the effects of strong electronic correlations on highly degenerate narrow band materials such as uranium and cesium based f-band metals. Short range ordering that may occur as a result of local moment correlations using a 1/N expansion, where N is the degeneracy of the material. Similar techniques applied to high $T_c$ superconductors. Field dependence of the de Haas-van Alphen effect. Compton scattering and angle resolved photoemission spectra for the latter materials. Comparison of theory with these and other experimental observations.

## PRINCETON UNIVERSITY
**M-49 Guyot Hall**
**Princeton, NJ 08544-1033**

**385. THERMOCHEMISTRY OF PHASES RELATED TO OXIDE SUPERCONDUCTORS**
A. Navrotsky, Department of Geological and Geophysical Sciences
(609) 258-4674 01-3 $95,445

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

**386. CONSOLIDATION OF COLLOIDAL DISPERSIONS; FILTRATION/SEDIMENTATION, FLOCCULATION AND PHASE SEPARATION**
W. B. Russel, Department of Chemical Engineering
(609) 258-4590 01-3 $60,000 (18 months)

Processing colloidal dispersions to form solids with tailored morphologies, ranging from dense packing with random or ordered microstructures to highly porous fractals. Study of filtration of flocculated dispersions. Effects of interparticle attraction, applied pressure, and initial volume fraction. Phenomenological model capturing the strength of the particle network through a compressive yield stress. Consolidation of nanosized particles through osmotic forces due to dissolved polymer. Assembly of particles with interesting electronic properties into order dense phases.

## PURDUE UNIVERSITY
**1021 Hovde Hall**
**West Lafayette, IN 47907**

**387. BEAM LINE OPERATION AND MATERIALS RESEARCH UTILIZING NSLS**
G. L. Liedl, Materials Engineering Division
(317) 494-4100 01-1 $273,612

A grant to support MATRIX, a group of scientists from several institutions who have common interests in upgrading and in utilizing X-ray synchrotron radiation for unique materials research. The group has available a specialized beam line at the National Synchrotron Light Source (NSLS). A unique and versatile monochromator provides radiation to a four-circle Huber diffractometer for the basic system. Multiple counting systems are available as well as a low temperature stage, a high temperature stage, and a specialized surface diffraction chamber. The grant covers the operational expenses and system upgrade of this beam line at NSLS for all MATRIX members, and to support part of the research on phase transformation studies, X-ray surface and interface studies.

**388. STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA**
H. Sato, School of Materials Engineering
(317) 494-4099 01-3 $82,430

The Cluster Variation Method (CVM) is being applied to the calculation of the percolation threshold in doped B-alumina. The CVM-PPM (Path Probability Method) is applied to chemical diffusion in multi-component systems. The frequency dependence of ionic conductivity, was also performed to understand the mechanism of the relaxation process generally observed in structurally disordered solid electrolytes.

**389. MIDWEST SUPERCONDUCTIVITY CONSORTIUM**
G. L. Liedl, Department of Materials Engineering and Physics
(317) 494-5567 01-5 $2,962,500

The Midwest Superconductivity Consortium (MISCON) was formed in response to Congressional direction. The consortium emphasis is in issues of ceramic superconductor synthesis, development, processing, electron transport, and magnetic behavior. Efforts are both theoretical and experimental. The membership includes Purdue University, Iowa State University, Notre Dame University, Ohio State University, Indiana University, and the University of Missouri-Columbia.

**390. GAMMA SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION**
J. R. Mullen, Department of Physics
(317) 494-3031 02-2 $75,000

This project aims at the development and use of ultra high intensity Mossbauer sources for scattering experiments. The technique has been shown to be feasible and it has been applied to the investigation of the precise character of the resonance line shape, anharmonicity in sodium, diffusive properties of organic liquids, and critical phenomena in charge density wave layer compounds. Studies have been initiated in soft modes, phasons and interference with potential applications in testing possible violation of time reversal invariance in the electromagnetic decay of nuclei. The work is being carried out at the University of Missouri Research Reactor Facility and with a specially constructured scattering facility at Purdue University. Both conventional and conversion electron scattering techniques are being used, particularly microfoil conversion electron (MICE) detectors to enhance signal-to-off-resonance counting rates. Strongly coupled to research of Dr. Yelon at the University of Missouri.

**391. ELECTRONIC AND STRUCTURAL PROPERTIES OF INDIVIDUAL NANOMETER-SIZE SUPPORTED METALLIC CLUSTERS**
R. G. Reifenberger, Department of Physics
(317) 494-3032    02-2 $62,000

Investigation of the photo-excitation process at low photon energies. Techniques under development directly measure the excited state energy distribution of electrons that are emitted through the surface potential barrier. The fundamental process is photo-excitation of electrons from field emission tips by a focussed argon-ion laser beam tuned to operate at a specific photon energy. Exploration of advantages and properties of a laser-illuminated scanning tunneling microscope. Technique of atomic force microscopy for determination of elastic properties of supported clusters.

## RENSSELAER POLYTECHNIC INSTITUTE
## Troy, NY 12180

**392. MECHANISM OF MECHANICAL FATIGUE IN FUSED SILICA**
M. Tomozawa, Department of Materials Engineering
(518) 276-6451    01-2 $82,430

Mechanism of cyclic fatigue and analysis of fatigue kinetics in fused silica. Measurement of diffusion coefficient and solubility of water in silica glass as a function of stress, temperature, and water vapor pressure. Preparation of silica glass containing various water contents. Effect of water content on swelling and mechanical property alteration. Effect of environment on crack initiation and propagation. Comparison of cyclic and static fatigue in various environments.

## UNIVERSITY OF RHODE ISLAND
**Kingston, RI 02881**

**393. SURFACE PHYSICS WITH COLD AND THERMAL NEUTRON REFLECTOMETRY**
A. Steyerl, Department of Physics
(401) 792-2204    02-1 $70,070 (10 months)

Extension of the methods of surface reflectometry with the use of ultra cold neutrons, which increases the experimental senstivity to the point where extremely small momentum and energy transfers relevant in critical surface phenomena. The ultracold neutron techniques with X-ray and thermal neutron reflectometry, as well as other techniques should lead to a more complete picture of surface properties. The techniques for this work require the development of high precision neutron optics. These developments will be exploited eventually at the Advanced Neutron Source.

## RICE UNIVERSITY
**Houston, TX 77251**

**394. APPLICATION OF SPIN-SENSITIVE ELECTRON SPECTROSCOPIES TO INVESTIGATIONS OF ELECTRONIC AND MAGNETIC PROPERTIES OF SOLIDS**
G. K. Walters, Department of Physics
(713) 527-6046

F. B. Dunning, Department of Physics
(713) 527-3544    02-2 $198,000

Spin-sensitive surface spectroscopies are being used to investigate electron inelastic scattering mechanisms and probing depths in metals, the electronic and magnetic properties of surfaces and thin films, the morphology of monolayer-level metal films, electron tunneling and surface states and the dynamics of metastable atom deexcitation and ion neutralization at surfaces. Spin Polarized Low Energy Electron Diffraction (SPLEED), Metastable Deexcitation Spectroscopy (MDS) and other evolving novel spin-polarized spectroscopic techniques provide required experimental tools. A spin-polarized $He^+$ ion beam and a superthermal $He(2_3S)$ metastable atom source will be developed.

## UNIVERSITY OF ROCHESTER
**Rochester, NY 14627**

**395. MICROSTRUCTURAL BEHAVIOR OF NON-EQUILIBRIUM SYSTEMS**
J. C. M. Li, Department of Mechanical Engineering
(716) 275-4038    01-2 $90,049

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

**396. DYNAMICS OF SURFACE MELTING**
H. E. Elsayed-Ali, Laboratory for Laser Energetics
(716) 275-5101 03-3 $85,000

Experimental study of the melting transition of metal single crystals focusing on the occurrence and nature of surface melting. Picosecond time resolved reflection high energy electron diffraction (RHEED) will be used as a surface structure probe. The fast time resolution will be used to examine the dynamical processes taking place during the melting transition. Picosecond laser heating will be employed. Initially, low index facets of lead, bismuth, zinc and cadmium will be examined.

## ROCKWELL INTERNATIONAL
**1049 Camino Dos Rios**
**Thousand Oaks, CA 91360**

**397. MECHANISMS OF MECHANICAL FATIGUE IN CERAMICS**
B. N. Cox, Science Center
(805) 373-4128

D. B. Marshall, Science Center
(805) 373-4170 01-2 $102,893

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

## RUTGERS STATE UNIVERSITY OF NEW JERSEY
**Piscataway, NJ 08854**

**398. MULTICOMPONENT GLASS SURFACES: STRUCTURE AND ADSORPTION**
S. H. Garofalini, Department of Ceramics
(908) 932-2216 01-3 $103,252

Molecular dynamic simulation of multicomponent glass surfaces, adsorption behavior and thin film formation using classical multibody and Embedded Atom Method (EAM) potentials and quantum chemical Car-Parrinello techniques. Experimental surface analysis with XPS, Ion Scattering Spectroscopy (ISS) and atomic force microscopy (AFM). Silicate glasses containing alkali metals, alkaline earths and network forming cations such as Al, Ti or B; adsorbates include Pt or Au, or reactive species such as Al or Ti.

**399. THERMODYNAMICS, KINETICS AND STRUCTURAL BEHAVIOR OF SYSTEMS WITH INTERMEDIATE PHASES**
A.G. Khachaturyan, Department of Mechanics and Materials Science
(908) 932-4711

T. Tsakalakos, Department of Mechanics and Materials Science
(908) 932-4711 01-1 $120,040

Elastic strain energy of an arbitrary two-phase microstructure. Strain-induced interaction of finite elements of a precipitate phase. Microscopic nonlinear kinetic equations of diffusional ordering with elastic strain contribution. Computer simulation of the strain-induced mesoscale structure in Y-Ba-Cu high-temperature superconducting oxides.

## UNIVERSITY OF SOUTHERN CALIFORNIA
**Los Angeles, CA 90089**

**400. FACTORS INFLUENCING THE FLOW AND FRACTURE OF SUPERPLASTIC CERAMICS**
T. G. Langdon, Department of Materials Science
(213) 740-0491 01-2 $100,000

Superplastic flow in ceramics; role of grain boundaries; yttrium oxide-tetragonal zirconia polycrystalline (Y-TZP) ceramics; grain-boundary glassy phase. Relationship between stress and strain rate as function of temperature and stresses, threshold stress; interrelationship between value of stress exponent, impurity level, and area fraction of intergranular glassy phase; effect of grain size on strain rate and activation energy; factors influencing tensile elongation to failure; cavitation.

**401. SYNTHESIS OF NOVEL ASSOCIATING WATER-SOLUBLE COPOLYMERS**
T. E. Hogen-Esch, Department of Chemistry
(213) 740-5980

E. J. Amis, Department of Chemistry
(213) 743-6913 03-1 $85,681

Synthesis of water-soluble acrylic and cellulosic copolymers based on perfluorocarbon- and polydimethyl-siloxane derivatives of acrylic comonomers in which the hydrophobe length and that of a flexible polyethylene oxide connecting spacer to the acrylic group are systematically varied. Structural features, important for enhancing the viscosity of aqueous solutions at very low polymer concentrations (<1000 ppm), will be investigated with dynamic light scattering, rheology and solution dynamics. The potential for mobility control of water-soluble copolymers that cluster as a result of polyanion-polycation interactions will be explored.

## SOUTHWEST RESEARCH INSTITUTE
**6220 Culebra Road**
**San Antonio, TX 78284**

**402. CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION**
R. A. Page, Department of Materials and Mechanics
(512) 522-3252

K. S. Chan, Department of Materials and Mechanics
(512) 522-2053 01-2 $103,000

Characterization of pore evolution during sintering and cavitation during creep. Objectives of the sintering study are the statistical characterization of pore evolution during densification, identification of primary variables affecting pore removal, and development and evaluation of sintering models. Objectives of the creep study are to understand the effects of microstructural parameters and loading mode, including uniaxial tension, on the kinetics of various creep mechanisms, such as grain boundary sliding and cavity growth. Small angle neutron scattering (SANS) measurements (supplemented by TEM, SEM, precision density, and AES characterization), tensile-creep measurements, and grain boundary sliding measurements (using stereo-imaging technique). Cavity size, distribution, morphology, and nucleation and growth rates determined by SANS analysis. Materials investigated included alumina and silicon carbide.

## SRI INTERNATIONAL
**Menlo Park, CA 94025**

**403. FUNDAMENTAL STUDIES ON PASSIVITY AND PASSIVITY BREAKDOWN**
D. D. Macdonald, Chemistry and Chemical Engineering Laboratories
(415) 859-3195

M. Urquidi-Macdonald, Chemistry and Chemical Engineering Laboratories
(415) 859-3195 01-3 $184,033

Study effects of minor alloying elements on passivity breakdown and of photo effects on the properties of passive films. Use electrochemical and photoelectrochemical techniques to explore the transport and kinetic properties of vacancies and change carriers in the films and at the metal/film and film/solution interfaces.

## STANFORD UNIVERSITY
**Stanford, CA 94305-2205**

**404. MECHANICAL PROPERTIES OF MULTILAYER THIN FILMS AND INTERFACES**
W. D. Nix, Department of Materials Science and Engineering
(415) 725-2605 01-2 $140,005

Study of the strength and adhesion properties of thin films and metal multilayers. FCC/BCC metal multilayer combinations with a wide range of wavelenghts made by sputter deposition. X-ray diffraction studies and substrate curvature measurements of multilayer stresses and TEM for the study of microstructure, defects and interfacial epitaxy. Nanoindentation substrate curvature measurements and bulge testing using a laser interferometer system. Modeling of the strength properties of metal multilayers.

**405. FUNDAMENTAL STUDIES OF THE CHEMICAL VAPOR COMPOSITION OF DIAMOND**
D. A. Stevenson, Department of Materials Science and Engineering
(415) 723-4251 01-3 $54,230 (18 months)

A study of the mechanism of growth of diamond coatings by enhanced chemical vapor deposition (ECVD). Primary emphasis on: a.) influence of enhancement methods (hot filament with and without DC bias), b.) rate of etching of graphite and diamond by atomic hydrogen, and c.) relation between gas phase chemistry and diamond coating. Coating process characterization by optical and mass spectroscopy methods; coatings characterized by RHEED, Raman spectroscopy, SIMS, SEM, TEM, XRD, profilometry, hardness, laser scattering and hot-stage stress measurements.

**406. ULTRA-LOW TEMPERATURE PROPERTIES OF AMORPHOUS SOLIDS**
D. D. Osheroff, Department of Physics
(415) 723-4228 02-2 $112,000

The thermal and dielectric properties of disordered solids between 1 mK and 100 mK are being investigated. The nature and role of lattice defects-two level systems-in the behavior of amorphous solids are being examined. Current thermometer technology is being extended in the temperature range of interest through a systematic investigation of the ultra-low temperature behavior of the dielectric constant of glasses.

**407. A QUEST FOR A NEW SUPERCONDUCTING STATE**
J. P. Collman, Department of Chemistry
(415) 723-4648

W. A. Little, Department of Physics
(415) 723-4233    03-1 $80,000 (6 months)

Research to understand the mechanism whereby high temperature superconductivity occurs in ceramic cuprates such as $YBa_2Cu_3O_7$ and related substances. A new experimental technique "gap modulation spectroscopy" is being used to study superconducting thin films as prepared by magnetron sputtering, laser ablation or other techniques. This technique allows the study of small changes in reflectivity due to variation of the gap function with temperature of current. X-ray diffraction results on copper free, superconducting bismuthate materials will be studied above and below $T_c$ searching for a structural phase transition-superconducting mechanism connection. A major focus of the work is the study of the newly discovered proximity effect to probe the nature of the superconducting state.

## STATE UNIVERSITY OF NEW YORK AT BUFFALO
**Buffalo, NY 14214**

**408. SUNY BEAMLINE FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE**
P. Coppens, Department of Chemistry
(716) 831-3911    02-2 $280,000

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 investigators from many of the State University of New York campuses, Alfred University, E. I. DuPont de Nemours, the Geophysical Institution and collaborative work with numerous other institutions. The research interests are: structure of materials, electronic structure of materials, surface physics, compositional analysis, and time-dependent biological phenomena.

**409. X-RAY STUDIES OF MICROSTRUCTURES IN SEMICONDUCTORS AND SUPERCONDUCTING MATERIALS**
Y. H. Kao, Department of Physics and Astronomy
(716) 636-2576    02-2 $100,937 (2 months)

Investigation of the short range order structure in semiconductors and high temperature superconducting materials. Experimental methods: X-ray fluorescence, absorption, scattering, and electron yield to probe the local environment surrounding impurity atoms, interfaces and depth profile of constituent atoms at the National Synchrotron Light Source at Brookhaven National Laboratory. High quality samples prepared and characterized by collaborators at IBM and Philips Laboratories.

## STATE UNIVERSITY OF NEW YORK AT STONY BROOK
**Stony Brook, NY 11794**

**410. ATOMIC AND ELECTRONIC STRUCTURE OF METALS AND ALLOYS - CLEAN SURFACES AND CHEMISORBED MOLECULES**
J. P. Jona, Department of Materials Science and Engineering
(516) 632-8508    02-2 $62,000

Investigation of the atomic and electronic structure of rare-earth metal surfaces, ultra-thin films of metals, and ordered surface alloys. Auger-electron spectroscopy used to monitor the chemical composition, and to determine cleanness of the respective samples. The surface region atomic geometry of the materials will be determined by qualitative and quantitative low-energy electron diffraction (LEED). In order to study the electronic band structure, ultraviolet photoemission spectroscopy (UPS), will be initilized both in the angle-integrated and in the angle-resolved mode.

**411. PHASE TRANSITION IN POLYMER BLENDS AND STRUCTURE OF IONOMERS**
B. Chu, Department of Chemistry
(516) 632-7928    03-2 $85,000

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

## UNIVERSITY OF UTAH

**309 Park Building**
**Salt Lake City, UT 84112**

**412. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS AND ORDERING IN III/V SYSTEMS**

G. B. Stringfellow, Department of Materials Science and Engineering
(801) 581-8387 01-1 $84,841

Explore the growth, ordering, and stability of III/V semiconducting alloys, with large positive enthalpies of mixing, prepared by organometallic vapor phase epitaxy (OMVPE). Emphasis on expanding the ordered structure domain size and increasing the degree of ordering. Characterization of structural, electrical, and optical properties by electron microscopy, electron microprobe, X-ray diffraction, photoluminescence, optical absorption, Raman spectroscopy, Hall effect, van der Pauw, conductivity, and magnetoresistance measurements. Computer modeling/simulation of growth and stabilities of these structures. Materials for study include alloys of GaAsSb, GaInAsSb, GaPSb, InPSb, and InAsSb.

**413. FABRICATION, PHASE TRANSFORMATION STUDIES, AND CHARACTERIZATION OF SIC-ALN-AL2OC**

A. V. Virkar, Department of Materials Science and Engineering
(801) 581-5396 01-1 $71,001

Analysis of phase equilibria and phase transformations and the relationship between creep behavior and microstructure in the SiC-AlN-$Al_2OC$ system. Diffusional phase transformations leading to phase separation. Modulated microstructures developed by spinodal decomposition. Cellular precipitation. Dependence of creep behavior on composition and microstructure.

**414. ALUMINA REINFORCED TETRAGONAL ZIRCONIA (TZP) COMPOSITES**

D. K. Shetty, Department of Materials Science and Engineering
(801) 581-6449 01-2 $79,827

Transformation toughening and reinforcement in composites; modeling of dependence of fiber-matrix interfacial properties on thermal expansion mismatch and processing temperature with glass-matrix composites; relationship between matrix cracking stress and interfacial properties. Effect of secondary additives on transformation toughening of Ce-TZP-alumina composites. Effects of fiber coatings on interfacial bonding and mechanical properties of alumina fiber-reinforced Y-TZP composites. Electrical-mechanical analog to evaluate stress-intensity factors for matrix cracks in fiber reinforced composites.

**415. PHOTOMODULATION SPECTROSCOPY OF PHOTOCARRIER DYNAMICS, ELECTRONIC DEFECTS AND MORPHOLOGY OF CONDUCTING POLYMER THIN FILMS**

Z. V. Vardeny, Department of Physics
(801) 581-8372 03-2 $102,000

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

## VIRGINIA COMMONWEALTH UNIVERSITY

**Richmond, VA 23284-2000**

**416. STRUCTURE, STABILITY AND SPECTROSCOPY OF METAL CLUSTERS**

P. Jena, Department of Physics
(804) 367-1313

B. K. Rao, Department of Physics
(804) 257-1313 01-3 $181,934

Theoretical studies of the evolution of atomic and electronic structure of Fe, Cu, Ni, and Al neutral and anionic clusters, and on hydrogenation of cluster vs. crystals. Construction of many-body potentials from ab initio Born-Oppenheimer energy surfaces of small clusters and their use in molecular dynamics simulation. Equilibrium geometries of large clusters using the simulated annealing method and model many-body potentials.

## VIRGINIA STATE UNIVERSITY

**Petersburg, VA 23803**

**417. CHARACTERIZATION OF SUPERCONDUCTING MATERIALS WITH MUON SPIN ROTATION**

C. E. Stronach, Department of Physics
(804) 524-5915 01-3 $239,578 (17 months)

Use of muon spin rotation to characterize the magnetic states in high temperature and heavy-fermion superconductors. Investigate the relationship between magnetic ordering and superconductivity.

## UNIVERSITY OF VIRGINIA
**Charlottesville, VA 22906**

**418. HETEROGENEOUS NUCLEATION IN METAL ALLOYS**
G. J. Shiflet, Department of Materials Science
(906) 487-2630 01-1 $98,916

Characterize active heterogeneous nucleation sites and preferred growth centers at these sites in metal alloys. Primary experimental techniques include isothermal heat treatments, and conventional, and high resolution electron microscopy. Because of what remains a lacuna in simulation of conventional two-beam TEM observations, dynamical calculations are a significant part of the current program. The most fundamental studies will involve coherent nucleation of $Al_3Li$ on matrix dislocations. Theories due to Cahn and Larche will be tested, and perhaps extended, to understand nucleation kinetics. Growth models will be developed to attempt to understand the unusual morphologies observed.
Semi-quantitative analysis will be applied to grain boundary nucleation in Al-Cu and Al-Cu-Mg systems to further examine nucleation at grain boundaries with and without trace elements.

**419. SURFACE STRUCTURE AND ANALYSIS WITH SCANNING TUNNELING MICROSCOPY AND ELECTRON TUNNELING SPECTROSCOPY**
R. V. Coleman, Department of Physics
(804) 924-3781 02-2 $130,000

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

**420. SUPERCONDUCTING MATERIALS**
J. Ruvalds, Department of Physics
(804) 924-3781 02-3 $50,000 (6 months)

Investigations of high temperature superconductors with emphasis on copper oxide alloys. The key features of the electron spectrum in these materials will be studied in order to identify the charge carriers. Emphasis on quasiparticle damping in view of the anomolous damping observed experimentally and calculated by the principal investigator. Normal state properties of the high temperature oxides will be investigated, including e.g., reflectively, the Hall effect, electronic Raman scattering, and anomolous susceptibility.

## WASHINGTON STATE UNIVERSITY
**Pullman, WA 99164-2920**

**421. METAL INDUCED EMBRITTLEMENT**
R. G. Hoagland, Department of Mechanical and Metallurgical Engineering
(509) 335-8280 01-2 $114,436

Study of embrittlement of metals and alloys by liquid metals. Effects of microstructure and strength on slow crack growth behavior. Fracture path characterization. Calculations of atomic behavior at crack tips. Effect of environment on ductile vs brittle behavior.

## WASHINGTON UNIVERSITY
**St. Louis, MO 63130**

**422. MULTI-BODY FORCES AND ENERGETICS OF TRANSITION METALS, ALLOYS, AND SEMICONDUCTORS**
A. E. Carlsson, Department of Physics
(314) 889-5739 02-3 $76,600

Development of computational methods for calculation of interatomic potentials used in simplified tight-binding models of transition metals and their alloys. Extension beyond the tight-binding model. Interatomic potentials tested both by experimental data and density-of-states band calculations. Applied to surfaces and vacancies and subsequently used to calculate phase diagrams and the properties of dislocations and grain boundaries.

## UNIVERSITY OF WASHINGTON
**Seattle, WA 98195**

**423. X-RAY AND GAMMA-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE**
R. L. Ingalls, Department of Physics
(206) 543-2778 02-2 $118,750

Investigate the structure and properties of materials at high pressures using X-ray absorption fine structure (XAFS) and gamma-ray (Mossbauer) spectroscopy. Emphasis on the study of materials undergoing pressure-induced phase transitions such as the bcc to hcp transformation in metallic iron and structural plus valence changes, such as in $TlReO_4$. The effects of pressure on the local structure of high temperature superconductors will also be examined. Mossbauer work is aimed at characterizing the recently discovered enhanced absorption of hydrogen by metallic iron at high pressures.

**424. THEORETICAL STANDARDS OF XAFS**
J. J. Rehr, Department of Physics
(206) 543-8593 02-2 $43,625

A state-of-the-art computer code for theoretical simulations of X-ray absorption fine structure (XAFS) for use by the XAFS community will be developed. The code will be consistent with recommendations of the International Workshop on Standards and Criteria in X-ray absorption. The latest theoretical developments will be incorporated and the code will be compared with experiment to choose between alternative theoretical prescriptions. The code will incorporate multiple scattering effects which are important in the complex materials.

**425. XAFS INVESTIGATION OF PHASE TRANSITIONS**
E. A. Stern, Department of Physics
(206) 543-2023 02-2 $80,000

X-ray absorption (XAFS) and Mossbauer studies on phase transitions. Lattice instabilities, defect structures and deviations from average structure will be investigated in high-$T_c$ superconductors. The nucleation of melting at impurity sites in metals such as Pb and Ag with a variety of impurities will be examined. Structural phase transitions in perovskites will be studied to observe the local structure and determine the phase transition mechanisms.

## UNIVERSITY OF WISCONSIN AT MADISON
**1509 University Avenue**
**Madison, WI 53706**

**426. THERMODYNAMIC AND KINETIC STABILITIES OF TWO-PHASE SYSTEMS INVOLVING GALLIUM ARSENIDE AND AN INTERMETALLIC PHASE**
Y. A. Chang, Department of Materials Science and Engineering
(608) 262-0389 01-3 $77,915

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

**427. LOCALIZED-ITINERANT MAGNETISM: THIN FILMS AND HETEROSTRUCTURES**
M. Onellion, Department of Physics
(608) 263-6829 02-2 $64,430

Application of the Magneto-Optic Kerr Effect (MOKE) with energies between 1.4 and 35 eV and electron spin polarization to the characterization of rare earth films, rare earth-transition metal bilayers and to chromium dioxide/cobalt heterostructures. Determination of rare earth core level anisotropy as a function of temperature and layer thickness. Investigation of the orientation of magnetism in rare earth thin films. Examine magnetic exchange interaction within and between layers in metal hetoersturcture.

**428. MORPHOLOGICAL ANALYSIS OF IONOMERS**
S. L. Cooper, Department of Chemical Engineering
(608) 262-4502 03-2 $46,250 (6 months)

This program involves the study of the bulk morphology relaxation mechanisms and solution properties of ion containing polymers. Synthesis of ionomers with regular placement of ionic groups along the chain. Small angle X-ray scattering techniques used to probe shape, size, and arrangements of ionic aggregates in ionomers. Effect of casting solvent, compression molding and solution casting on morphology. Anomalous small angle X-ray scattering (ASAXS) to resolve source of zero-angle upturn in scattering intensity. Tensile properties to monitor the dramatic cation influence, the effect of water, trends within a chemical group and the effect of anion type. SANS experiments using deuterated polyols will measure temperature dependence, response to deformation and be interpreted for cation effects.

## UNIVERSITY OF WISCONSIN AT MILWAUKEE
**Milwaukee, WI 53201**

### 429. INELASTIC ELECTRON SCATTERING FROM SURFACES
S. Y. Tong, Department of Physics
(414) 229-5765 02-3 $96,000

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 of the University of California at Irvine.

### 430. UNDULATOR SPECTRO-MICROSCOPY FACILITY AT THE ADVANCED LIGHT SOURCE
B. P. Tonner, Department of Physics
(414) 229-4626 02-2 $100,000

Support for the design and construction of a beamline at the ALS light source. This includes the design, construction and commissioning of: 1) a photoelectron diffraction and holography station, 2) a scanning photoemission microscope (SPEM), 3) a fluorescence spectrometer, and 4) a multilayer optics X-ray beam splitter. The SPEM will have a spatial resolution close to the diffraction limit of 200nm which is 5 times greater than the current state-of-the-art instrument. The spectral resolution of the instrument will be a greater than 0.1 eV. Specifications for the holography and photoelectron diffraction systems will be drawn up. Complete ray tracing for the beamline will be performed to determine the optimal configuration for the SPEM optics.

## YALE UNIVERSITY
**New Haven, CT 06520**

### 431. MICROSTRUCTURAL DEPENDENCE OF THE CAVITATION DAMAGE POLYCRYSTALLINE MATERIALS
B. L. Adams, Department of Mechanical Engineering
(203) 432-0159 01-2 $81,100

Establish microstructural and stress state dependence of cavitation damage in F.C.C. metal alloys. Experimental and analytical studies will define a Cavitation-Damage Function under multi-axial loading. The technique involves measuring local crystallite orientations adjacent to grain boundaries of sectioned samples using Electron Backscattering Diffraction. Type 304 stainless steel and copper alloys will be studied.

# SECTION C

Small Business Innovation Research

## ADVANCED TECHNOLOGY MATERIALS, INC.
**7 Commerce Drive**
**Danbury, CT 06810**

**432. A NOVEL FABRICATION METHOD FOR DIAMOND COMPOSITES**
P. Chen
(203) 794-1100 Phase I SBIR $50,000 (6 months)

Diamond and copper are unique in their ability to efficiently conduct heat, making them premier materials for electronic applications for which heat removal is critical to system performance. Differences in their other properties make it attractive to combine these two materials into a diamond/copper composite that has improved properties over those of copper alone. Diamonds offer a cost-effective means of improving thermal of copper. In this project, the feasibility of fabricating near net shapes of dimaond/copper composites is being investigated. The thermal and mechanical properties of the resulting composites are being determined for evaluation of the material's utility in electronic and space thermal management applications.

## INRAD, INC.
**181 Legrand Avenue**
**Northvale, NJ 07647**

433. SINGLE CRYSTAL MOLYBDENUM MIRROS FOR HIGH POWER X-RAY SYNCHROTRONS
W. Ruderman
(201) 767-1910 Phase I SBIR $499,026

Synchrotrons are being used increasingly for scientific research and for X-ray lithography for the production of high-density memory chips. This has created a need for mirrors capable of withstanding the high synchrotron X-ray flux. Molybdenum has many of the properties that are needed for mirrors, such as high melting point, hardness, high structural strength, high figure of merit for thermal distortion, and high reflectance for X-rays. In addition, single crystals are superior to polycrystalline molybdenum because they can be ion-beam polished and have a higher thermal conductivity. Conventional crystal growth methods are not suitable for making the large area crystals required for synchrotron mirrors. Phase I research has led to a novel technique for productiong large aspheric mirrors that will be made from a polycrystalline molybdenum substrate whose upper surface will consist of high quality single crystal molybdenum. This technique will be applicable to a wide range of other mirror materials that are stable at their melting point. Phase II of this project will further develop a novel zone surface crystal growth process to produce single crystal material for large synchrotron mirrors. Another objective is to further develop the polishing process to produce superpolished crystal surfaces. Crystals will be characterized with respect to crystal perfection, surface flatness and roughness, and subsurface damage. Reflectance measurements for X-ray engines from 100 eV to 10 keV will be made for representative samples at the National Synchrotron Light Soruce at Brookhaven National Laboratory. Anticipated Results/Potential Commercial Applications as described by the awardee: The availability of large, high quality, single-crystal molybdenum mirrors will be very important for synchrotrons used for scientific research and for the emerging X-ray lithography needs of the semiconductor industry.

## IONWERKS
**2215 Addison**
**Houston, TX 77030**

**434. IN SITU SURFACE ELEMENTAL ANALYSIS/PROCESS CONTROL AT MILLITORR PRESSURE DURING SUPERCONDUCTOR FILM DEPOSITION**
J. A. Schultz
(713) 522-9800 Phase I SBIR $50,000 (6 months)

The high pressure limits of a new proprietary technique for surface elemental and isotopic analysis are being explored. The technique will be useful in the millitor pressure regime, thus allowing measurement of thin film stoichiometry during growth and processing. The present research is focussing on analysis of yttrium-barium-copper-oxygen (YBCO) superconductor films subjected to high pressures of oxygen. In Phase I, the technique is being calibrated using standard YBCO surfaces, its high pressure limit is being determined, and real-time measurement of substrate/thin film interdiffusion is being attempted.

## JET PROCESS CORPORATION
**25 Science Park**
**New Haven, CT 06511**

**435. CONTROL OF THIN FILM MICROSTRUCTURES BY GAS DYNAMIC ENERGY DEPOSITION**
B. Halpern
(203) 786-5130 Phase I SBIR $50,000 (6 months)

An influence on the microstructure of thin films can be obtained during film growth by energy deposition at the surface. A new approach to energy deposition is made possible by the jet vapor deposition (JVD) technique: the impact of gas dynamically accelerated neutral atoms and molecules. This technique employs supersonic inert jets in low vacuum fast flows as high throughout, environmentally sound deposition sources for metals, semiconductors, dielectrics, and organics in multicomponent, alloy, or multilayer form. Energies of this magnitude promote surface mobility and defect-free deposition. One jet is used to deposit and a second jet to "impact anneal" a film moving periodically past both jets. Bombarded and unbombarded films will be compared in order to demonstrate the benefits of coupling low temperature film growth with low temperature, gas dynamic energy deposition.

## MULTILAYER OPTICS AND X-RAY TECHNOLOGY, INC.
**7070 University Station**
**Provo, UT 84602**

**436. WAVELENGTH DISPERSIVE X-RAY SPECTROMETERS FOR ANLYATICAL TRANSMISSION ELECTRON MICROSCOPY**
M. W. Lund
(801) 378-3972 Phase II SBIR $500,000

In Phase I, techniques to make X-ray reflectors on flexible substrates were developed. In Phase II these reflectors will be used to develop two complementary wavelength dispersive spectrometers. The first is a sequential spectrometer similar to the Johann and Johannson types, but with greater collection efficiency and simplified mechanical construction. The other is a parallel detection wavelength dispersive X-ray spectrometer which has lower collection efficiency, but can accurately and simultaneously measure X-ray peak height ratios. Anticipated Results/Potential Commercial Applications as described by the awardee: There are important problems in energy, biology, environmental quality, and materials science for which existing analytical transmission electron microscopy X-ray analysis equipment is inadequate. The current techniques are energy dispersive spectroscopy (EDS) and electron energy loss spectroscopy (EELS). Wavelength dispersive spectrometers offer 15 times better resolution, 10 times better peak-to-background ratio than EDS. Wavelength dispersive spectrometery will complement EDS and EELS is allowing convenient, high accuracy analyses of light elements under conditions where such analyses are not now possible.

## NANODYNE, INC.
**11 Industrial Drive**
**New Brunswick, NJ 08901**

**437. A GENERIC CHEMICAL PROCESSING TECHNOLOGY FOR THE PRODUCTION OF NANOSTRUCTURED COMPOSITE MATERIALS**
L. E. McCandlish
(908) 249-8347 Phase I SBIR $49,823 (6 months)

Spray conversion processing (SCP) is a new chemical processing technology capable of producing bulk quantities of nanostructured composite powders, staring from water soluble precursors. The technology has considered versatility, but is unable to deal with reactive elements such as aluminum (Al), silicon (Si), titanium (Ti), vanadium (V), niobium (Nb), and tantalum (Ta), which form thermodynamically stable oxides that cannot this project is studying the incorporation of chemical vapor infiltration (CVI) of reactive elements as a final step in the SCP of high surface area (nanoporous) powders. Nanostructured tungsten carbid-cobalt (WC-Co) powders with 30 to 50 nm WC grain size have been produced successfully by SCP. However, during consolidation by liquid-phase sintering, the WC grain size rapidly coarsens to about 200 to 300 nm, even after a short time (5 min) at the peak sintering temperature (1,400°C). The primary objective of this research is to achieve a further reduction in WC grain size in the fully consolidated materials by making use of a known grain growth inhibitor, vanadium carbide (VC).

## PEAK INSTRUMENTS, INC.
**112 West Franklin Ave.**
**Pennington, NJ 08534**

**438. AN EFFICIENT X-RAY WAVELENGTH SPECTROMETER FOR IMPROVED ELEMENTAL ANALYSIS ON ELECTRON MICROSCOPES**
N. C. Barbi
(609) 737-8133 Phase II SBIR $399,601

A new type of wavelength dispersive (WD) X-ray spectrometer is being developed. Its anticipated attributes include (1) high efficiency with high resolution; (2) small physical size; and (3) high-vacuum compatability. Phase I results showed improvements that potentially enable wavelength spectroscopy to be performed on several types of electron microscopes (EMs) currently unsuitable for WD spectrometers: (1) analytical electron microscopes (AEMs), which require a great reduction is spectrometer size; (2) large-chamber scanning electron microscopes (SEMs), which require larger Rowland circles than presently available or are likely to become available (owing to reduced efficiency); (3) cold field-emission SEMs, which, owing to low total beam current, require higher efficiency than is now delivered; and (4) field-emission instruments or any other type of EM requiring higher vacuum levels, which are inherently incompatible with large volume spectrometer housings and gas-flow proportional counters. Calculations in Phase I, based primarily on the ability to significantly reduce crystal-to-sample distance, predict potential efficiency gains for the new device of typically 1 to 2 orders of magnitude over conventional WD systems. Compared to energy dispersive spectrometers commonly used on all of the above instruments, the new spectrometer will provide more sensitive analysis, particularly for the light elements. Anticipated Results/Potential Commercial Applications as described by the awardee: The result of this project will be the development of a compact efficient wavelength dispersive spectrometer system for potential applicaton on AEMs and large-chamber and field emissions SEMs. The commercial applications include improved elemental analysis on these types of instruments, particularly for the light elements.

## POLARIS RESEARCH

**P. O. Box 24**
**Saratoga, CA 94071**

**439. FAST-PULSE HOT PRESSING WITH FINE-SCALE ADIABATIC HEATING**
M. D. Matthews
(408) 261-2803 *Phase I SBIR $48,972 (6 months)*

The planned process development relates to fast-pulse hot pressing using input power densities on the order of a gigawatt/cc. Power inputs of this magnitude can produce adiabatic heating on a fine scale in mixtures of dielectric and conductive powders. Melting of the conductive phase with minimal heat loss to the dielectric phase during heating allows for consolidation under pressure in a very short time, with minimum energy equilibrium temperature is considerably lower than the melting point of the conductive phase, enabling the use of high pressures and low-cost materials to construct the equipment. The project is investigating graphite/diamond and boron carbid/titanium nitride as possible materials system. A polycrystalline diamond compact can probably be produced through rapid heating and cooling at pressures below the equilibrium pressure for diamond. The materials are fully consolidated and studied by X-ray diffraction, the phases are identified, and key mechanical properties are measured.

## PSI TECHNOLOGY COMPANY

**20 New England Bus. Ctr.**
**Andover, MA 01810**

**440. PRODUCTION OF CONTROLLED MICROSTRUCTURE NANOPHASE CERAMIC POWDERS**
J. J. Helble
(508) 689-0003 Phase I SBIR $50,000 (6 months)

The fabrication of advanced ceramic materials from ultrafine, nanometer-size grains, "nanophase materials," has the potential to signficantly enhance ceramic properties. This project investigates a novel aerosol process for the general production of multicomponent, unagglomerated ceramic oxide powders. Yttria-stabilized zirconia with 10 to 40 nm grains will be produced to demonstrate process feasibility. Sintering tests on a pellet produced from this powder will then be conducted to assess energy savings (reductions in sintering temperature) resulting from the nanometer-scale grain structure.

## QUANTUM MAGNETICS, INC.

**11578 Sorrento Valley Rd.**
**San Diego, CA 92121**

**441. DUCTILE HIGH-TEMPERATURE SUPERCONDUCTING ALLOYS**
R. E. Sager
(619) 481-4015 Phase I SBIR $49,804 (6 months)

The brittleness and low critical current densities of high-temperature superconducting (HTS) compounds are serious impediments to component fabrication and the ultimate commericialization of these materials. This project explores and further develops a novel processing technique for HTS materials conceived at the University of California/San Diego (UCSD). This technique is designed to address the problems of HTS utilization by forming ductile HTS oxide-silver alloys through controlled oxidation from precursor materials. The feasibility of a new diagnostic tool will be demonstrated (an ultrahigh vacuum (UHV) - compatible superconducting quantum interference device (SQUID) magnetometer) that, in close collaboration with UCSD, will allow the continued development and eventual commericialization of this new process. The program includes the fabrication of very high quality alloy precursor materials as films, characterization of their superconducting properties, establishment of a UHV capability for testing SQUIDs, and an investigation of the electrical properties of metal-HTS contacts important in microelectronic applications.

## X-RAY INSTRUMENTATION ASSOCIATES

1300 Mill Street
Menlo Park, CA 94025-3210

**442. DIGITAL PROCESSING ELECTRONICS FOR X-RAY DETECTOR ARRAYS**

W. K. Warburton
(415) 903-9980 Phase I SBIR $50,000 (6 months)

Many areas of synchrotron radiation investigation are severely detector limited, particulary in cases where single photon, energy dispersive counting is required. Because the maximum count rate for a single detector at a given energy resolution is limited, arrays of detectors are being constructed to increase total count rates. This approach is not restricted by the cost, physical size, and complexity of the required analog processing electronics. Initial studies have investigated the possibility of developing digital processing electronics based on concepts of digital signal processing. These studies suggest that it should be possible to match the resolutions of current analog systems while increasing processing speeds by factors of 2 to 6 and decreasing both costs and physical sizes by an order of magnitude. This project's over-all goal is to determine whether it is actually possible to construct such digitally based signal processing systems. In particular, this work aims to identify optimum filter designs, evaluate the performance of these filters with real pre-amplifiers, and develop an implementable design using commercially available hardware to the greatest extent possible.

## X-RAY OPTICAL SYSTEMS

1400 Washington Avenue
Albany, NY 12222

**443. A COLD/THERMAL BEAM BENDER USING CAPILLARY OPTICS TO INCREASE THE NUMBER OF END-GUIDE INSTRUMENT POSITIONS**

Q. Xiao
(518) 442-5250 Phase I SBIR $50,000 (6 months)

The development and use of nondestructive, neutron-based analytical techniques for materials characterization-including neutron-scattering applications using cold and thermal neutrons have been hindered by limited access to high flux sources of low energy neutrons. This project is developing a device that would transmit a wide wavelength range of cold and thermal neutrons through a small radius of curvature, enabling the creation of several end positions on a single neutron guide. The resulting beams would be essentially free of contamination from epithermal neutrons and gamma-rays. The neutron beam bender would consist of any array of capillaries with small diameter channels through which the neutrons would make multiple reflections at angles less than the critical angle of reflection. Such capillary-based devices, referred to as Kumakhov optics, have demonstrated the capability redirect X-rays.

# SECTION D

Major User Facilities

(Large Capital Investment)

# INTENSE PULSED NEUTRON SOURCE

**Argonne National Laboratory**
**Argonne, Illinois 60439**

IPNS is a pulsed spallation source dedicated to research on condensed matter. The peak thermal flux is $4 \times 10^{14}$ n/cm$^2$ sec. The source has some unique characteristics that have opened up new scientific opportunities:

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

Two principal types of scientific activity are underway at IPNS: neutron diffraction, concerned with the structural arrangement of atoms (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties, and inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level. At the same time, the facilities are used for technological applications, such as stress distribution in materials and characterization of zeolites, ceramics, polymers, and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS, Building 360, Argonne National Laboratory. Neutron time for proprietary research can be purchased based on the full-cost recovery rate.

PERSONS TO CONTACT FOR INFORMATION

B. S. Brown, Division Director (708) 252-4999
Argonne National Laboratory FAX (708) 252-4163
IPNS Building 360
9700 South Cass Avenue
Argonne, IL 60439

T. G. Worlton, Scientific Secretary (708) 252-8755

# IPNS EXPERIMENTAL FACILITIES

| Instrument (Instrument Scientist) | Range Wave-vector* (Å$^{-1}$) | Range Energy (eV) | Resolution Wave-vector (Å$^{-1}$) | Resolution Energy (eV) |
|---|---|---|---|---|
| Special Environment Powder Diffractometer (J. D. Jorgensen/R. Hitterman) | 0.5-50 | ** | 0.35% | ** |
| General Purpose Powder Diffractometer (J. Richardson/R. Hitterman) | 0.5-100 | ** | 0.25% | ** |
| Single Crystal Diffractometer (A. J. Schultz/R. Goyette) | 2-20 | ** | 2% | ** |
| Low-Res. Medium-Energy Chopper Spectrometer (R. Osborn/L. Donley) | 0.1-30 | 0-0.6 | 0.02 $k_o$ | 0.05 $E_o$ |
| High-Res. Medium-Energy Chopper Spectrometer (C.-K. Loong/J. Hammonds) | 0.3-9 | 0-0.4 | 0.01 $k_o$ | 0.02 $E_o$ |
| Small Angle Diffractometer (J. E. Epperson/P. Thiyagarajan/ D. Wozniak) | 0.006-0.35 | ** | 0.004 | ** |
| Low-Temperature Chopper Spectrometer (P. E. Sokol - Penn State University, (814) 863-0528) | 0.3-30 | 0.1-0.8 | 0.01 $k_o$ | 0.02 $E_o$ |
| Polarized Neutron Reflect. (POSY) (G. P. Felcher/R. Goyette) | 0.0-0.07 | ** | 0.0003 | ** |
| Neutron Reflect. (POSY II) (W. Dozier/R. Goyette) | 0.0-0.25 | ** | 0.001 | ** |
| Quasi-Elastic Neutron Spectrometer Spectrometer (F. Trouw) | 0.42-2.59 | 0-0.1 | ~0.2 | 70 μeV<-><br>0.01ΔE |
| Glass, Liquid and Amorphous Materials Diffractometer ℜ (D. L. Price/K. Volin) | 0.05-25<br>01-45 | **<br>** | ~0.5% cotθ<br>~1.0% cotθ | **<br>** |
| High Intensity Powder Diffractometer (F. Trouw) | 0.5-25<br>1.8-50 | **<br>** | 1.8-3.5%<br>0.9% | **<br>** |

* Wave-vector, $k = 4\pi \sin\theta/\lambda$.
** No energy analysis.
ℜ Two sample positions
<-> Elastic and inelastic resolution

**Not Yet in the User Program**
**Small Angle Neutron Diffractometer (SAND, formerly SAD II, under development)**

# HIGH FLUX BEAM REACTOR

**Brookhaven National Laboratory**
**Upton, New York 11973**

The Brookhaven High Flux Beam Reactor (HFBR) presently operates at a power of 30 megawatts and provides an intense source of thermal neutrons (total thermal flux = $1.0 \times 10^{15}$ neutrons/cm$^2$-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($\gamma > 4$ A). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure is also available. The emphasis of the research efforts at the HFBR has been on the study of fundamental problems in the fields of solid state and nuclear physics and in structural chemistry and biology.

USER MODE

Experiments are selected on the basis of scientific merit by a Program Advisory Committee (PAC), composed of the specialists in relevant disciplines from both within and outside BNL. Use of the facilities is divided between Participating Research Teams (PRT's) and general users. PRT's consist of scientists from BNL or other government laboratories, universities, and industrial labs who have a common interest in developing and using beam facilities at the HFBR. In return for their development and management of these facilities, each PRT is assigned up to 75 percent of the available beam time, with the remainder being reserved for general users. The PAC reviews the use of the facilities by the PRT's and general users and assigns priorities as required.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/ student research groups performing experiments at the National Synchrotron Light Source or at the HFBR. It is aimed at university users having limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

Rae Greenberg (516) 282-5564
Bldg. 510A Fax (516) 282-5888
Brookhaven National Laboratory
Upton, NY 11973

# HIGH FLUX BEAM REACTOR (continued)

## TECHNICAL DATA

| INSTRUMENTS | PURPOSE AND DESCRIPTION |
|---|---|
| 5 Triple-axis Spectrometers (H4M, H4S, H7, H8, H9A) | Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 MeV, < $E_o$ < 200 MeV Q range: 0.03 < Q < $10_{A-1}$ |
| Small Angle Neutron Scattering (H9B) | Studies of large molecules. Located on cold source with 20 x 20 $cm^2$ position-sensitive area detector. Sample detector distance L < 2 meter. Incident wavelength 4 Å < $\lambda_o$ < 10 Å |
| Diffractometer (H3A) | Protein crystallography 20 x 20 $cm^2$ area detector $\lambda_o$ = 1.57 Å |
| Small Angle Scattering (H3B) | Studies of small angle diffraction of membranes. Double multilayer monochromator 1.5 Å < λ < 4.0 Å 2d detector with time slicing electronics and on-line data analysis. |
| 2 Diffractometers (H6S, H6M) | Single-crystal elastic scattering 4-circle goniometer 1.69 Å < $\lambda_o$ < 0.65 Å |
| 1 Triple-axis Spectrometer (H5) | Inelastic scattering<br>Diffuse scattering<br>Powder diffractometry |
| 2 Spectrometers (H1A, H1B) | Neutron capture studies Energy range: 0.025 eV < $E_o$ < 25 KeV |
| <u>TRISTAN II (Isotope Separator)</u> (H2) | Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission |
| <u>Irradiation Facilities</u> | |
| 7 Vertical Thimbles | Neutron activation; production of isotopes; thermal flux: 8.3 x $10^{14}$ neutrons/$cm^2$-sec; fast (> 1.0 MeV) flux: 3 x $10^{14}$ neutrons/$cm^2$-sec. |
| <u>Instruments - Soon to be Commissioned</u><br>Neutron Reflectometer | Accommodates liquid or solid samples up to 40 cm long. $.0025Å^{-1} \leq Q \leq 0.25Å^{-1}$, with resolution 1 x $10^{-3}Å^{-1}$. Reflection range $1\text{-}10^{-6}$. |
| High Resolution Neutron Powder Diffractometer. (H1A1) | Determination of moderately complex crystalline structures. λ = 1.88Å, Δd/d = 5 x $10^{-4}$Ge(511) vertical focussing |

# NATIONAL SYNCHROTRON LIGHT SOURCE

**Brookhaven National Laboratory**
**Upton, New York 11973**

The National Synchrotron Light Source (NSLS) is the nation's largest facility dedicated to the production of synchrotron radiation. The facility has two electron storage rings: a vacuum ultraviolet ring which operates at an electron energy of 0.75 GeV and an X-ray ring which operates at 2.5 GeV. The bending magnet sources on these rings provide useable photon fluxes from 0.01 to 1.0 keV and 1.0 to 20.0 keV, respectively. These bending magnets are the source for the 30 X-ray ports and 17 VUV ports. By further sharing of these sources, as many as four beamlines can be accommodated on a single port, providing the NSLS facility with a capacity to run approximately 101 experiments simultaneously. By the end of 1991, the Light Source had 82 operational beamlines conducting experiments.

From their conception, the designs of the storage rings included long, field free straight sections for special radiation sources (wigglers and undulators). The two straight sections on the VUV ring and the five available on the X-ray ring now have a variety of wigglers and undulators providing radiation that is anywhere from one to several orders of magnitude brighter than the comparable bending magnets. These devices are the sources for a wide variety of experiments in the biological, chemical, and materials sciences.

Photons, as a probe, provide information about the electronic and atomic structures of interest to the chemical, biological, and materials sciences. The techniques fall broadly into two areas: spectroscopy and scattering. At the NSLS, they are applied to forefront research: imaging in both real space (e.g., X-ray, microscopy tomography, angiography) and reciprocal space (e.g., protein crystallography, X-ray topography), surface science (e.g., photoemission, surface diffraction, infrared spectroscopy), and recently magnetism (e.g., magnetic X-ray scattering, magnetic circular dichroism, and spin polarized photoemission). These are but a few of the exciting research opportunities at the NSLS. In July 1992, 2,500 scientists from 390 universities, laboratories, corporations, and foreign institutions were registered at the Light Source. Nine Hundred students were pursuing graduate and post-graduate studies at the NSLS in 1992.

Proprietary research can be performed at the NSLS. The DOE has granted the NSLS a Class Waiver under whose terms the Proprietary User is obligated to pay the full cost recovery rate for NSLS usage. In return, the user has the option to take title to any inventions made during the proprietary research program and to treat as proprietary all technical data generated during the proprietary research program. In FY 1991, the total number of corporations participating in proprietary research at the Light Source was six.

## USER MODES

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in establishment of comprehensive long-range experimental programs. In addition to the beamlines constructed by the NSLS staff for general usage, a large number of beamlines have been designed and instrumented by Participating Research Teams (PRTs). The PRTs are entitled to up to 75 percent of their beamline(s) operational time for a 3-year term.

Insertion Device Teams (IDTs) have been formed to design, fabricate, commission, and use wiggler and undulator beamlines. The conditions and terms are similar to those of the PRTs.

General users are scientists interested in using existing NSLS facilities for experimental programs. General User proposals are reviewed and those accepted are scheduled by an independent beamtime allocation committee for a percentage of operating time for each beamline. Liaison and utilization support is provided to the General User by the cognizant beamline personnel. Two hundred nineteen new General User proposals were submitted during FY 1991. A total of 1,961 days of beam time was allocated to General Users on the X-ray and VUV rings during FY 1991.

A program is available to support faculty/student research groups performing experiments at the NSLS. The program is designed to encourage new users of these facilities and defray expenses incurred during exploratory visits to BNL, and while conducting initial experiments at the NSLS. It is aimed at university users having only limited grant support for their research. Sixty-eight scientists, 30 faculty, and 38 students representing 20 universities participated in this program in FY 1991. One hundred eight institutions have now participated in this program since its inception in 1984.

PERSON TO CONTACT FOR INFORMATION

Susan White-DePace
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# NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

## TECHNICAL DATA

| Storage Ring | Key Features | Operating Characteristics |
|---|---|---|
| VUV electron | High brightness; continous wavelength range ($E_c$25Å);17 ports | 0.75 GeV electron energy |
| X-ray electron | High brightness; continous wavelength range ($E_c$25Å); 30 beam ports | 2.5 GeV electron energy |

| Research Area | Wavelength Range (Å) | Energy Range (eV) | Number of Instruments |
|---|---|---|---|
| Circular Dichroism | 1400 - 6000 | 2.1 - 8.9 | 1 |
| Energy Dispersive Diffraction | WB; 0.1 - 103 | WB; 120 - 100,000 | 3 |
| EXAFS, NEXAFS, SEXAFS | WB; 0.4 - 2480 | WB; 5 - 35,000 | 19 |
| Gas Phase Spectroscopy/ Atomic Physics | WB; 0.6 - 6.2 | WB; 2000 - 20,000 | 3 |
| High Pressure Physics | 0.1 (Å) - 10,000 (μm) | 0.12 (meV) - 100,000(eV) | 3 |
| Infrared Spectroscopy | 2.5 (μm) - 10,000 (μm) | 0.12 (meV) - 490 (meV) | 1 |
| Lithography/Microscopy/ Tomography/Radiography | WB; 0.1 - 124 | WB; 3 - 100,000 | 10 |
| Medical Research | WB; 0.3 - 3.1 | WB; 4000 - 36,000 | 3 |
| Nuclear Physics | — | 80 - 400 (meV) | 1 |
| Photoionization | 0.6 - 4000 | 3 - 20,000 | 2 |
| Radiometry | WB; 8.3 - 248 | WB; 50 - 1,500 | 1 |
| Reflectometry | 20 (Å) - 10,000 (μm) | 0.12 (meV) - 620 (eV) | 2 |
| Research and Development/ Diagnostics | WB | WB | 12 |
| Time Resolved Fluorescence | 350 - 6000 | 2.1 - 35 | 2 |
| Topography | WB; 0.1 - 3.1 | WB; 4000 - 100,000 | 3 |
| VUV and X-ray Photoemission Spectroscopy | 0.3 - 6199 | 2.0 - 40,000 | 27 |
| X-ray Crystallography | 0.1 - 6.2 | 2000 - 100,000 | 10 |
| X-ray Fluorescence | WB; 0.1 - 620 | WB; 20 - 100,000 | 4 |
| X-ray Scattering/ Diffraction | WB; 0.1 - 6.2 | WB; 2000 - 100,000 | 28 |
| X-ray Standing Wave | WB; 0.4 - 4.1 | WB; 3000 - 34,000 | 2 |

WB = White Beam

# LOS ALAMOS NEUTRON SCATTERING CENTER

**Los Alamos National Laboratory**
**Los Alamos, New Mexico 87545**

The Los Alamos Neutron Scattering Center (LANSCE) facility is a pulsed spallation neutron source equipped with time-of-flight (TOF) spectrometers for condensed-matter research. Neutrons are produced by spallation when a pulsed 800-MeV proton beam, provided by the Los Alamos Meson Physics Facility (LAMPF) and an associated Proton Storage Ring (PSR), impinges on a tungsten target. To date, the PSR has achieved 75 percent of its design goal of 100-μA average proton current at 20-Hz repetition rate. At this level, LANSCE has the world's highest, peak thermal flux for neutron scattering research.

Current research programs at LANSCE use the following instruments: a filter difference spectrometer (FDS) for vibrational spectroscopy by inelastic neutron scattering; a Laue-TOF single-crystal diffractometer (SCD); a high-intensity powder diffractometer (HIPD) for structural studies of liquids, amorphous materials, and crystalline powders; a neutron powder diffractometer (NPD) with the highest resolution in the U.S.; a constant-Q spectrometer (CQS) for the study of collective excitations, such as phonons and magnons; a low-Q diffractometer (LQD) for small-angle scattering studies; and a surface profile reflectometer (SPEAR) for studies of surface structure.

During the next 3 to 4 years, several new spectrometers will be installed at LANSCE, including: a chopper spectrometer for inelastic scattering measurements and Brillouin scattering and a back-scattering spectrometer with a resolution of 10 μeV or better.

USER MODE

LANSCE provides neutron scattering facilities for several communities. At least 80 percent of available beam time is used for condensed-matter research, while the remaining 20 percent is intended for internal use in support of the Laboratory's programmatic mission. Of the time available for condensed- matter work, most is distributed to a formal user program, which started in April 1988. Advice on experiments to be performed in this category is provided by a Program Advisory Committee (PAC) held jointly with the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory. Scientists based at universities, national laboratories, and industry may apply for beam time by submitting short proposals for scrutiny by the PAC. No charge is made for non-proprietary research.

CONTACT FOR USER INFORMATION

Maria DiStravolo (505) 667-6069
LANSCE Scientific Coordination and Liaison Office
Mail Stop H805
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

# LOS ALAMOS NEUTRON SCATTERING CENTER (continued)

## TECHNICAL DATA

| | |
|---|---|
| Proton Source | LAMPF + PSR |
| Proton Source Current | 1000 μA |
| Proton Source Energy | 800 MeV |
| LANSCE Proton Current | 75 μA |
| Proton Pulse Width | 0.27 μs |
| Repetition Rate | 20 Hz |
| Epithermal Neutron Current (n/eV.Sr.S) | $3.2 \times 10^{12}/E$ |
| Peak Thermal Flux ($n/cm^2.S$) | $1.7 \times 10^{16}$ |

### INSTRUMENTS

| | |
|---|---|
| 32-m Neutron Powder Diffractometer<br>(J. Goldstone, Responsible) | Powder Diffraction<br>Wave vector 0.3-50 $Å^{-1}$<br>Resolution 0.13% |
| Single Crystal Diffractometer<br>(A. Larson, Responsible) | Laue time-of-flight diffractometer Wave vectors 1-15 $Å^{-1}$<br>Resolution 2% typical |
| Filter Difference Spectrometer<br>(J. Eckert, Responsible) | Inelastic neutron scattering, vibrational spectroscopy<br>Energy trans. 15-600 meV<br>Resolution 5-7% |
| High Intensity Powder Diffractometer<br>(R. VonDreele, Responsible) | Powder diffraction .7% resolution; liquids and amorphous materials diffraction 2% resolution |
| Constant-$\underline{Q}$ Spectrometer<br>(R. Robinson, Responsible) | Elementary excitations in single crystal samples<br>Energy resolution 1-3% |
| Low Q Diffractometer<br>(P. A. Seeger, Responsible) | Small angle scattering at a liquid hydrogen cold source<br>Wave vectors 0.003-1.0 $Å^{-1}$ |
| Reflectometer<br>(G. Smith, Responsible) | Surface reflection at grazing incidence. Wave vector range 0.007 to 0.3 $Å^{-1}$ |

# NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

**Solid State and Chemistry Divisions**
**Oak Ridge National Laboratory**
**Oak Ridge, Tennessee 37831**

The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, phase transitions, crystal structures, polymers, micelles, ferrofluids, ceramics, and liquid crystals. The HFIR is an 85-MW, light-water moderated reactor. The central flux is $4 \times 10^{15}$ neutrons/cm$^2$-sec, and the flux at the inner end of the beam tubes is slightly less than $10^{15}$ n/cm$^2$-sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Facilities are available for studies of materials at low and high temperatures, high pressures, and high magnetic fields.

## USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an external review committee. It is expected that all accepted experiments will be scheduled within 6 months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be borne by the user. 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<br>Solid State Division<br>Oak Ridge National Laboratory<br>Oak Ridge, Tennessee 37831-6393 | (615) 574-5240 | Wide Angle |
| G. D. Wignall<br>Solid State Division<br>Oak Ridge National Laboratory<br>Oak Ridge, TN 37831-6393 | (615) 574-5237 | Small Angle |

# NEUTRON SCATTERING AT THE HIGH FLUX ISTOTOPE REACTOR (continued)

## TECHNICAL DATA

| | |
|---|---|
| HB-1 | Triple-axis polarized-beam, Beam size - 2.5 by 3 cm max, Flux - 2.6 x $10^6$ n/cm$^2$s at sample (polarized), Vertical magnetic fields to 5 T, Horizontal fields to 2 T, Variable incident energy ($E_o$) |
| HB-1A | Triple-axis, fixed $E_o$, $E_o$ = 14.7 MeV, Wavelength = 2.353 angstroms, Beam size - 5 by 3.7 cm max, Flux - 9 x $10^6$ n/cm$^2$s at sample with 40 min collimation |
| HB-2, HB-3 | Triple-axis, variable $E_o$, Beam size - 5 x 3.7 cm max, Flux - $10^7$n/cm$^2$sat sample with 40 min collimation |
| HB-3A | Double-crystal small-angle diffractometer, Beam size - 4 x 2 cm max, Wavelength = 2.6 angstroms, Flux - $10^4$ n/cm$^2$s, Resolution - 4 x $10^{-5}$ angstroms$^{-1}$ |
| HB-4A | Wide-angle time-slicing diffractometer, Beam size - 2 x 3.7 cm max, Wavelength = 1.537 angstroms, Flux - 2 x $10^6$ n/cm$^2$s with 9 min collimation, Curved linear position sensitive detector covering 130° |
| HB-4 | Correlation chopper, Beam size - 5 x 3.7 cm, Flight path - 1.5 m, 70 detectors covering 130°, Variable $E_o$, Variable pulse width<br><br>Powder Diffractometer, Beam size - 5 x 3.7 cm, Wavelength = 1.4 angstroms, 32 detectors with 6 min collimators |
| HB-4SANS | Small-Angle Scattering Facility, Beam size - 3 cm diameter max, Wavelength = 4.75 or 2.38 angstroms, $10^4$ - $10^6$ n/cm$^2$s depending on slit sizes and wavelength, area detector 64 x 64 cm$^2$, sample to dector distance 1.5 - 19 m |

# STANFORD SYNCHROTRON RADIATION LABORATORY

**Stanford University**
**Stanford, California 94309-0210**

SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research in biology, chemistry, engineering, geology, materials science, medicine and physics. In addition to scientific research utilizing synchrotron radiation the Laboratory program includes the development of advanced sources of synchrotron radiation (e.g., insertion devices for the enhancement of synchrotron radiation as well as modifications of SPEAR). SSRL presently has 24 experimental stations. The radiation on 12 stations is enhanced by insertion devices providing some of the world's most intense X-ray sources.

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. X-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter. X-ray lithography and microscopy. SSRL serves approximately 650 scientists from 114 institutions working on over 150 active proposals. A wide variety of experimental equipment is available for the user and there are no charges either for use of the beam or for the facility-owned support equipment. Proprietary research may be performed on a cost-recovery basis by special arrangement.

USER MODE

SSRL is a user-oriented facility which welcomes proposals for experiments from all qualified scientists. SSRL operates for users 7-8 months per year. Over 75 percent of the beam time is available for the general user. Access is gained through proposal submittal and peer review. An annual Activity Report is available on request. It includes progress reports on about 100 experiments plus descriptions of recent facility developments. The booklets "Proposal Submittal and Scheduling Procedures" and "SSRL Experimental Stations" detail information on proposal submittal and experimental station characteristics.

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell (415) 926-3191
SSRL, 69 PO Box 4349 M.S.
Stanford, CA 94309-0210

# SECTION E

Other User Facilities

# MATERIALS PREPARATION CENTER

**Ames Laboratory**
**Iowa State University**
**Ames, Iowa 50011**

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section, the Materials Referral System and Hotline (MRSH), and the High-$T_c$ Superconductivity Information Exchange. The Analytical Section has extensive expertise and capabilities for the characterization of materials, including complete facilities for chemical and spectrographic analyses, and selected services of this section are available to the research community. The purpose of MRSH is to accumulate information from all known National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community. The High-$T_c$ Superconductivity Information Exchange provides a centralized site for rapid dissemination of up-to-date information on high- temperature superconductivity research. It publishes the newsletter, <u>High-$T_c$ Update</u>, twice-monthly without charge, as both hard copy and electronic mail.

## USER MODE

### Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Frederick A. Schmidt, Director, or Lawrence L. Jones, Associate Director, Materials Preparation Center.

### Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquiries should be directed to Tom Wessels, MRSH Manager, (515) 294-8900.

### High-$T_c$ Superconductivity Information Exchange

The newsletter, <u>High-$T_c$ Update</u>, is published twice-monthly and available without charge as either hard copy or electronic mail. Inquiries should be directed to Ellen O. Feinberg, (515) 294-3877.

# MATERIALS PREPARATION CENTER (continued)

## 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
Ames Laboratory
Materials Preparation Center
121 Metals Development Building
Ames, Iowa 50011

Lawrence L. Jones, Associate Director (515) 294-9808
Ames Laboratory
Materials Preparation Center
114 Metals Development Building
Ames, IA 50011

# 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 Corporation 2 MV Tandem Ion Accelerator and a NEC 650 kV Ion Injector which can produce ion beams from 10 keV to 8 MeV of most stable elements in the periodic table. 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 (High Resolution Electron Microscope (JEOL 4000 EXII), a JEOL I00 CXII transmission and scanning transmission electron microscope (TEM/STEM) equipped with an X-ray energy dispersive spectrometer (XEDS), a Philips EM 420 TEM/STEM equipped with XEDS and an electron energy loss spectrometer (EELS) and a Philips CM30 with XEDS. Installation of a VG6032 advanced Analytical Electron Microscope (AEM) is underway. This state-of-the-art, field emission gun ultra-high vacuum AEM will operate up to 300 keV and have the highest available microanalytical resolution with capabilities for XEDS, EELS, and Auger Electron Spectroscopy AES. As such, it will have substantially increased analytical capabilities for materials research over present-day instruments.

## USER MODE

The HVEM-Tandem Facility is operated as a national resource for materials research. Qualified scientists wishing to conduct experiments using the HVEM/TANDEM facilities of the Center should submit a proposal to the person(s) named below. Experiments are approved by a Steering Committee following peer evaluation of the proposals. There are no use charges for basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

## PERSON(S) TO CONTACT FOR INFORMATION

C. W. Allen (708) 252-4157
and
E. A. Ryan (708) 252-5075
Electron Microscopy Center for Materials Res.
Materials Science 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<br>Kratos/AEI EM7 (1.2 MeV) | Resolution 9 Å pt-pt<br>Continuous voltage selection (100-1200 kv)<br>Current density 15 A/cm$^2$<br>High-vacuum specimen chamber<br>Negative-ion trap<br>Electron and ion dosimetry systems<br>Video recording system<br>Ion-beam interface<br>Specimen stages 10 - 1300 K<br>Straining and environmental stages |
| Transmission Electron Microscope<br>JEOL 100 CX (100 keV) | Resolution 7 Å pt-pt<br>Equipped with STEM, XEDS<br>Specimen stages 85 - 900 K |
| Transmission Electron Microscope<br>Philips EM 420 (120 keV) | Resolution 4.5 Å pt-pt<br>Equipped with EELS, XEDS<br>Specimen stages 30 - 1300 K |
| Transmission Electron Microscope<br>Philips CM 30 (300 keV) | Resolution 2.5 Å pt-pt<br>Equipped with XEDS<br>Specimen stages 30 - 1300 K |
| High Resolution Electron Microscope<br>JEOL 4000 EXII (400 kV) | Resolution 1.65 Å pt-pt<br>Specimen stages RT |
| Analytical Electron Microscope<br>VG6032 being installed (300 keV) | Resolution 2.8 Å pt-pt<br>Ultra-high vacuum, Field Emission Gun<br>Equipped with EELS, XEDS, AES, SIMS, LEED, etc.<br>Specimen stages 85 - 1300 K |

| ACCELERATORS | |
|---|---|
| NEC Model 2 UDHS | Terminal voltage 2 MV<br>Energy stability ± 250 eV<br>Current density: $H^+$, 10 $\mu$A/cm$^2$<br>(typical) $Ni^+$, 3 $\mu$A/cm$^2$ |
| NEC 650 kV Injector<br>Being acquired | Terminal voltage 650 kV<br>Energy stability ± 60 eV<br>Current density: $He^+$, 100 $\mu$A/cm$^2$<br>(typical) $Ar^+$, 10 $\mu$A/cm$^2$ |

# CENTER FOR MICROANALYSIS OF MATERIALS

**Materials Research Laboratory**
**University of Illinois**
**Urbana-Champaign, Illinois 61801**

The Center operates a wide range of advanced microchemistry, surface chemistry, electron microscopy, X-ray and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, micro- crystallography, surface analysis, structure, etc. A team of professionals runs the facility and its members facilitate the research.

## USER MODE

Most of the research in the facility is funded from the MRL, DOE, and NSF contracts, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff. The Center welcomes external users from National Laboratories, Universities, and Industry.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research with a faculty member associated with the MRL. Independent usage by trained individuals is also encouraged. Assistance and collaboration with the professional staff of the Center is arranged as required. In all cases, the research carried out by users of the Center has to be in the furtherance of DOE objectives.

The equipment is made available on a flexible schedule. Professional help by the Center staff will be arranged to assist the users. Fully qualified users can and do use the equipment at any time of the day.

The Center staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

In addition to the main items listed opposite, the Center also has also equipment: optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including ion-milling stations, a micro-ion mill, electropolishing units, sputter coaters, a spark cutter, ultrasonic cutter, diamond saw, dimpler, etc.

## PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217) 333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

# CENTER FOR MICROANALYSIS OF MATERIALS (continued)

| INSTRUMENTS | 'ACRONYM' | FEATURES AND CHARACTERISTICS |
|---|---|---|
| Imaging Secondary Ion Microprobe Cameca IMS 5f | SIMS | Dual ion sources ($Cs^+$, $O_2^+$). 1 μm resolution. |
| Secondary Neutral Mass Spectrometer Leybold Heraeus INA 3 | SNMS | Quantitative analysis. Depth profiling. |
| Scanning Auger Microprobe Physical Electronics 595 | Auger | Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector. |
| Scanning Auger Microprobe Physical Electronics 660 | Auger | Resolution: SEM 25 nm Auger 60 nm |
| X-ray Photoelectron Spectrometer Electronics 5400 | XPS | Resolution: 50 meV, 180° Physical spherical analyzer, Mg/Al and Mg/Ag anodes |
| X-ray Photoelectron Spectrometer Surface Science | XPS | Spherical analyzer, small spot size, gas doping, high temperature |
| Transmission Electron Microscope Philips EM430 (300kV) | TEM | Heating and cooling stages |
| Transmission Electron Microscope Philips EM420 (120kV) Stage (30K). | TEM | EDS (windowless), EELS, STEM, Cathodoluminescence, Cold |
| Transmission Electron Microscope Philips EM400T (120kV) | TEM | EDS. Heating, cooling stages |
| Transmission Electron Microscope Philips CM12 (120 kV) | TEM | High Resolution Analytic facilities |
| Transmission Electron Microscope JEOL 4000EX (400 kV) | TEM | For environmental cell use. Straining stages, heating stages |
| Transmission Electron Microscope Hitachi 9000 (modified) | TEM | 0.16 nm resolution atomic imaging |
| Scanning Transmission E.M. Vacuum Generators HB5 (100kV) | STEM | 0.5 nm probe, field emission gun, EDS, EELS. |
| Scanning Electronic Microscope Hitachi S800 | SEM | Field Emission Gun Resolution 2nm, EDX |
| Scanning Electron Microscope EDX, JEOL JSM 35C (35kV) | SEM | 5 nm resolution, channeling and backscattering patterns. |
| Scanning Electron Microscope Zeiss 960 | SEM | High temperature deformation. Channeling, Backscattering, EDX, Electron beam lithography |
| Rutherford Backscattering (3 MeV) | RBS | Two work stations, channeling |

## CENTER FOR MICROANALYSIS OF MATERIALS (continued)

| INSTRUMENTS | "ACRONYM" | FEATURES AND CHARACTERISTICS |
|---|---|---|
| X-ray Equipment<br>Elliott 14 kW high brilliance source<br>Rigaku 12 kW source<br>Several conventional sources<br>Rigaku D/Max-11B Computer Controlled Powder Diffractometer | X-ray | 4-circle diffractometer.<br>Small angle camera. EXAFS.<br>Lang topography, Powder cameras, etc. High temperature and low temperature stages. |
| Proton Induced X-ray Emission | PIXE | Quantitative chemical analysis |
| Van de Graff Accelerator for electrons and ions | | 3 MeV accelerator<br>Rutherford Backscattering<br>Electron radiation damage<br>Ion radiation damage |

# 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 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 1.6MeV Kratos microscope dedicated largely to in situ work, a 1-MeV JEOL atomic resolution microscope with 1.5 angstrom point-to-point (ARM), a 200-kV high-resolution feeder microscope (JEOL 200 CX), and a 200-kV analytical microscope (JEOL 200 CX) equipped with a thin window and a high-angle X-ray detector, and an energy-loss spectrometer. Facilities for image simulation, analysis and interpretation are also available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. J. J. Hren, Chairman, D. G. Howitt, R. Geiss, D. J. Smith, T. L. Hayes, C. W. Allen, M. M. Treacy, and L. E. Thomas; internal members are G. Thomas, K. M. Krishnan, U. Dahmen, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be of sufficient merit can be carried out as a collaborative effort between a Center post-doctoral fellow, the outside proposer, and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Gretchen Hermes (510) 486-5006 or
*National Center for Electron Microscopy*
Mail Stop: 72-150
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

# NATIONAL CENTER FOR ELECTRON MICROSCOPY (continued)

## TECHNICAL DATA

| INSTRUMENTS | KEY FEATURES | CHARACTERIZATION |
|---|---|---|
| KRATOS 1.5-MeV Electron Microscope | Resolution 3 Å (pt-pt) environmental cell; hot stage, cold stage, straining stage, straining/heating stage, CBED, video camera, Faraday cup | 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 < 1.6 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, $\pm 40°$ biaxial tilt with height control. | 60 hrs/week, 400 kV-1 MeV, $LaB_6$ filament, 3-mm diameter specimens. |
| JEOL 200 CX Electron Microscope | Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only. | 200 kV only, $LaB_6$ filament, 2.3-mm or 3-mm diameter specimens. |
| JEOL 200 CX dedicated Analytical Electron Microscope | Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, PEELS spectrometer. | 100 kV-200 kV $LaB_6$ filament, state-of-the-art resolution; 3-mm diameter specimens. |

# SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

**Metals and Ceramics Division**
**Oak Ridge National Laboratory**
**Oak Ridge, Tennessee 37831**

A wide range of facilities for use in materials science are available for collaborative research by members of universities or industry with ORNL staff members. The facilities include state-of-the-art electron microscopy, high voltage electron microscopy, atom probe/field ion microscopy, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include analytical electron microscopy (energy dispersive X-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS), and convergent beam electron diffraction (CBED)). Surface analysis facilities include four Auger electron spectroscopy (AES) systems, and 0.4, 2.0, and 5.0 Van de Graaff accelerators for Rutherford back-scattering and nuclear reaction techniques. Other equipment includes a mechanical properties microprobe (Nanoindenter), X-ray diffraction systems, rapid solidification apparatus, and various other facilities in the Metals and Ceramics Division.

## USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, K. B. Alexender, G. M. Pharr, M. G. Burke, and N. D. Evans. 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
P. O. Box 2008
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 Capabilities | Applications |
|---|---|---|
| Philips EM400T/ FEG(AEM) 120 kV | EDS, EELS, CBED, STEM; minimum probe diam ~1 nm* | Structural and elemental microanalysis |
| Philips CM12 AEM 120kV | EDS, CBED, STEM;* | Structural and elemental microanalysis |
| JEOL 2000FX AEM 200 kV | EDS, CBED, EELS, STEM; examination of irradiated materials | Structural and elemental microanalysis |
| Philips CM30 AEM 300kV | EDS, (P) EELS, CBED, STEM; | Structural and elemental microanalysis |
| JEM 120C TEM 120 kV | Polepiece for TEM of ferromagnetic materials | Structural analysis |
| Atom Probe Field-Ion microscopes | TOF atom probe, imaging atom probe, FIM, pulsed laser atom probe | Atomic resolution imaging: single atom analysis elemental mapping |
| PHI 590 Scanning Auger Electron Spectroscopy System | 200 nm beam; fracture stage; RGA; depth profiling elemental mapping | Surface analytical and segregation studies |
| Varian Scanning Auger Electron Spectroscopy System | 5 micron beam; hot-cold fracture stage; RGA: depth profiling; elemental mapping | Surface analytical and segregation studies; gas-solid interaction studies |
| Triple Ion-Beam Accelerator Facilities | 400 kV, 2 MV, 5 MV Van de Graff accelerators sputter profiling | Nuclear microanalysis; Rutherford backscattering; elemental analysis |
| Mechanical Properties Microprobe-Nanoindenter | Computer-controlled diamond indenter | High spatial resolution (0.1 $\mu$m lateral and 0.2 nm depth) measurements of elastic/plastic behavior |

* Video recording; stages for cooling, heating, and deformation available for Philips microscopes.

# SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER

**Solid State Division**
**Oak Ridge National Laboratory**
**Oak Ridge, Tennessee 37831**

This program utilizes a new approach for fundamental materials research. Ion implantation doping, ion-induced mixing, and other ion beam based techniques are utilized to alter the near-surface properties of a wide range of solids under vacuum conditions. In situ analyses by ion beam, surface, and bulk properties techniques are used to determine the fundamental materials interactions leading to these property changes. Since ion implantation doping is a nonequilibrium processes, it can be used to produce new and often unique materials properties not possible with equilibrium processing. Ion beam techniques are also useful to modify surface properties for practical applications in areas such as friction, wear, corrosion, catalysis, surface hardness, solar cells, semiconducting devices, superconductors, etc.

This program has emphasis on long-range basic research. Consequently, most cooperative 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 many instances such research projects identify definite practical applications and accelerate the transfer of these materials alteration techniques to processing applications.

## COOPERATIVE RESEARCH

User interactions are through mutually agreeable 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
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6048

# SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER

## TECHNICAL DATA

| ACCELERATORS | OPERATING CHARACTERISTICS |
|---|---|
| 2.5-MV positive ion Van de Graaf | 0.1-3.2 MeV; H, O, $^{4}He$, $^{3}He$, and selected gases. Beam current 100 nA |
| 1.7-MV tandem | 0.2-3.5 MeV H; 0.2-5.1 MeV $^{3}He$, $^{4}He$; negative ion sputtering source for heavy ion beams of selected 7 MeV |
| 10-200-KV high-current ion implantation accelerator | Most ion species; 100-1000 microamps singly charged, microamps doubly and triply charged ~100 |
| 80-500-kV high-current ion implantation accelerator | Most ion species from microamp to milliamp current |

| FACILITIES | |
|---|---|
| UHV analysis chambers | Several chambers; vacuums $10^{-6}$-$10^{-11}$ torr; multiple access ports; UHV goniometers (4-1300K) |
| In situ analysis capabilities | Ion scattering, ion channeling, and ion-induced nuclear reactions; LEED, Auger, ion-induced Auger; electrical resistivity vs. temperature |
| Scanning electron microscope | JEOL-840 with energy dispersive X-ray analysis |
| Rapid thermal annealer | AG Heatpulse Model 410, with programmable, multistep heating to 1200° C. |

# DOE CENTER OF EXCELLENCE FOR THE SYNTHESIS AND PROCESSING OF ADVANCED MATERIALS

## SANDIA NATIONAL LABORATORIES ALBUQUERQUE, NEW MEXICO 87185

MEMBER LABORATORIES

Ames Laboratory, Argonne National Laboratory, Brookhaven National Laboratory, University of Illinois Materials Research Laboratory, Lawrence Berkeley Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest Laboratory, Sandia National Laboratories.

OBJECTIVE

The overall objective of this newly-established Center is to enhance synthesis and processing in the DOE with the objective of developing the technology base for the commercialization of new advanced materials.

Synthesis and processing (S&P) are those essential elements of materials science and engineering (MS&E) that deal with the assembly of atoms or molecules to form materials, the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and the development of processes to produce materials for specific applications. Clearly, S&P represent a large area of MS&E that spans the range from fundamental research to applied technology. The goal of basic research in this area ranges from the creation of new materials and the improvement of the properties of known materials, to the understanding of such phenomena as a diffusion, crystal growth, sintering, phase transitions, etc., in relation to S&P. On the applied side, the goal of S&P is to translate scientific results into useful materials by developing processes capable of producing high quality, low-cost products.

APPROACH

The Center's approach is to:

1. Support innovative, fundamental S&P research.
2. Emphasize the concurrent development of S&P including processing equipment and new instruments and techniques for real-time analysis and control.
3. Capitalize on the diverse interdisciplinary science and engineering expertise of the member laboratories.
4. Established partnerships among the Laboratories and Universities to capitalize on those strengths of Universities which complement and reinforce the Center's objectives.
5. Establish partnerships between the DOE labs and industry to demonstrate the ability to shorten the time between the generation and application of MS&E knowledge, to insure the selection of problems of genuine commercial value and to insert the technology into commercial manufacturing concerns.
6. Document the principles learned, the advances made and the remaining barriers.

# THE SYNTHESIS AND PROCESSING OF ADVANCED MATERIALS (continued)

In this approach, the emphasis will be on making the processes of basic research, development and applications engineering more concurrent, interactive and overlapping.

FOCUS AREAS

1. Atomically-Structured Materials
2. Complex Polymers
3. Advanced Ceramics and Ceramic Thin Films
4. Advanced Metals and Alloys
5. Emerging Materials and Processes

PERSON TO CONTRACT FOR INFORMATION

Geroge A. Samara (505) 844-6653
CAdvanced Materials Physics, 1153
Sandia National Laboratories
Albuquerque, New Mexico 87185

# COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

**Sandia National Laboratories**
**Livermore, California 94551-0969**

Optical techniques, primarily Raman spectroscopy and ultrafast nonlinear optical spectroscopy, are being developed and used to study the behavior of materials. Both pulsed and continuous-wave lasers at various wavelengths throughout the visible and ultraviolet regions are available for excitation of Raman scattering, which can be analyzed with 1 and 2 dimensional photon counting detectors, multichannel diode array detectors, and gated detection. Ultrahigh vacuum chambers and laboratory furnaces are available that are equipped with convenient optical access. Real-time measurements are complemented by post-exposure techniques such as Raman spectroscopy, sputtering and low-energy electron diffraction.

Amplified ultrashort-pulse lasers provide sub-one hundred femtosecond pulses at energies up to ten microjoules. Samples can be investigated under ambient conditions or at temperatures down to 4.8K. Analysis of samples in UHV-based systems provides careful control over the preparation and modification of surfaces. Laser ablation deposition is available for thin film growth of high-$T_c$ superconductors and other advanced ceramics.

USER MODE

Interactions include: (1) collaborative research projects with outside users, and (2) technology transfer of new diagnostic 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

R. H. Stulen, Advanced Materials Research Division (8342) — (510) 294-2070

Gary B. Drummond, Assistant to the Director (8301) — (510) 294-2697
Sandia National Laboratories
Livermore, California 94551-0969

# COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

## TECHNICAL DATA

| INSTRUMENTS | KEY FEATURES | COMMENTS |
|---|---|---|
| Raman Surface Analysis System | UHV Chamber; Raman system with Ar laser; triple spectrograph, diode array detector and 2-D imaging photon counting detector; Auger; sputtering capability. | Simultaneous Raman and sputtering. Raman system capable of detecting 2 nm thick oxides. Sample heating up to 1100 C. |
| Raman Microprobe | Hot stage; Raman system with Ar, Kr lasers; scanning triple spectrometer. | 1-2 micron spatial resolution. Hot stage can handle corrosive gases. |
| Raman High-Temperature Corrosion System | Furnace; Raman system with Ar, Kr, Cu-vapor lasers Nd:YAG; triple spectrograph and diode array detector. | Pulsed lasers gated detection for blackbody background rejection. Furnace allows exposure to oxidizing, reducing, and sulfidizing environments. |
| Combustion Flow Reactors | Raman system with Ar, Kr, Cu-vapor. lasers; triple spectrograph and diode array detector. | Vapor and particulate injection into flames. Real-time measurements of deposit formation. |
| Linear and Non-Linear Optical Spectroscopy of Electrochemical Systems | Electrochemical cell; Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and diode array detector; Nd:YAG laser, 1 Hz rep. rate. | Electrochemical cell with recirculating pump and nitrogen purge; Monolayer and submonolayer detection of metals, oxygen, and hydrogen adsorption at electrodes. |
| Nonlinear Optical Spectroscopy of Surfaces System | Picosecond Nd:YAG and dye lasers, 10 Hz; UHV chamber equipped with LEED, Auger, sputtering, and quad. mass spectroscopy; 100-ns pulse length, 10 Hz Nd:YAG laser. | Monolayer and submonolayer detection of high temperature hydrogen and oxygen adsorption and nitrogen segregation on alloys; laser thermal disorption. |
| Nonlinear Optical Spectroscopy of Electrochemical Systems | Ng-YAG laser, 1kHz rep rate; electrochemical cell. | Monolayer and submonolayer detection of metals, oxygen, and hydrogen adsorption at electrodes. |
| Ultrafast Optical Spectroscopy | Sub-100-fs CPM ring dye laser; copper-vapor-laser-pumped amplifier. | Transient absorption and transient grating experiments. |

# SECTION F

Summary of Funding Levels

# SUMMARY OF FUNDING LEVELS

During the Fiscal Year ending September 30, 1992, the Materials Sciences total support level amounted to about $257.1 million in operating funds (budget outlays) and $18.0 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. 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) | 37.7 | 25.0 |
| (b) South.................. (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV) | 9.2 | 20.9 |
| (c) Midwest................ (IA, IL, IN, MI, MN, MO, OH, WI) | 29.2 | 29.0 |
| (d) West................... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA) | 23.9 | 25.1 |
| | 100.0 | 100.0 |

2. By Discipline:

| | Grant Research (% by $) | Total Program (% by $) |
|---|---|---|
| (a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-) | 62.7 | 23.6 |
| (b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-) | 27.5 | 20.2 |
| (c) Materials Chemistry (Budget Activity Numbers 03-) | 9.8 | 7.8 |
| (d) Facility Operations | --- | 48.4 |
| | 100.0 | 100.0 |

# SUMMARY OF FUNDING LEVELS (continued)

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) | 22.1 |
| (b) DOE Laboratory Research Programs | 28.8 |
| (c) Major Facilities at DOE Laboratories | 47.4 |
| (d) Industry and Other | 1.7 |
| | 100.0 |

4. By Laboratory and Contract and Grant Research:

| | Total Program (%) |
|---|---|
| Ames Laboratory | 3.6 |
| Argonne National Laboratory | 18.7 |
| Brookhaven National Laboratory | 20.2 |
| Idaho National Engineering Laboratory | 0.2 |
| Illinois, University of (Materials Research Laboratory) | 2.6 |
| Lawrence Berkeley Laboratory | 13.6 |
| Lawrence Livermore National Laboratory | 0.9 |
| Los Alamos National Laboratory | 4.9 |
| National Renewable Energy Laboratory | 0.3 |
| Oak Ridge National Laboratory | 18.2 |
| Pacific Northwest Laboratory | 1.2 |
| Sandia National Laboratory | 3.1 |
| Stanford Synchrotron Radiation Laboratory | 1.0 |
| Contract and Grant Research | 11.5 |
| | 100.0 |

# SECTION G

Index of Investigators,

Materials, Techniques,

Phenomena, and Environment

# INVESTIGATOR INDEX

# MATERIALS, TECHNIQUES, PHENOMENA, AND ENVIRONMENT

The numbers in parenthesis at the end of each listing of Abstract numbers gives for each topic the percentage of prorated projects, the percentage of funding, and the percentage of individual projects respectively. The prorated projects and the funding levels are based on estimates of the fractions of a given project devoted to the topic. The operating funds for Fiscal Year 1992 were $257,111,000. The number of projects is 443.

## MATERIALS

Actinides-Metals, Alloys and Compounds

5, 14, 30, 32, 52, 133, 140, 154, 159, 161, 228, 282, 323, 362, 384
(0.97, 0.44, 3.39)

Aluminum and its Alloys

6, 17, 39, 52, 64, 69, 81, 114, 116, 117, 140, 157, 175, 188, 267, 268, 279, 318, 327, 343, 347, 418, 421
(1.20, 0.52, 5.19)

Alkali and Alkaline Earth Metals and Alloys

4, 39, 58, 180, 269
(0.25, 0.19, 1.13)

Amorphous State: Liquids

36, 56, 98, 103, 137, 141, 197, 222, 258, 291, 293, 294, 341, 364, 381
(1.02, 0.50, 3.39)

Amorphous State: Metallic Glasses

18, 22, 27, 53, 67, 69, 114, 123, 141, 148, 156, 180, 188, 211, 222, 249, 287, 332, 395
(1.06, 0.89, 4.29)

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

28, 76, 88, 141, 183, 186, 211, 222, 224, 225, 234, 252, 290, 294, 303, 340, 408
(0.84, 0.66, 3.84)

Amorphous State: Non-Metallic Glasses (Silicates)

15, 86, 154, 204, 210, 222, 225, 239, 252, 290, 294, 303, 332, 392, 398, 408
(1.13, 0.59, 3.61)

Carbides

15, 76, 80, 118, 140, 143, 144, 154, 182, 184, 190, 195, 196, 225, 234, 257, 263, 332, 343, 402, 413, 418, 439
(1.06, 0.65, 5.19)

Polymers

15, 20, 37, 40, 60, 92, 97, 100, 101, 105, 134, 135, 160, 164, 165, 171, 175, 181, 183, 188, 199, 200, 202, 207, 208, 244, 245, 246, 262, 263, 277, 289, 295, 321, 334, 335, 338, 357, 358, 376, 382, 400, 406, 407, 408, 411, 415, 428
(3.84, 1.60, 10.84)

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

11, 24, 71, 99, 114, 117, 140, 144, 220, 254, 265, 272, 283, 299, 350, 426
(0.63, 0.28, 3.61)

Quantum Fluids and Solids

12, 28, 98, 121, 123, 130, 163, 164, 180, 251, 292, 314
(0.95, 0.46, 2.71)

Radioactive Waste Storage Materials (Hosts, Canister, Barriers)

86, 187, 228, 340, 374
(0.59, 0.25, 1.13)

Rare Earth Metals and Compounds

1, 2, 5, 7, 8, 10, 11, 14, 18, 30, 52, 53, 55, 116, 123, 133, 140, 159, 161, 162, 164, 180, 261, 280, 282, 337, 383, 420, 427
(1.72, 1.25, 6.55)

Refractory Metals (Groups VB and VI B)

2, 3, 8, 11, 18, 19, 22, 65, 71, 140, 149, 160, 184, 190, 227, 277, 328, 341, 433
(1.08, 0.85, 4.29)

Superconductors - ceramic (also see superconductivity in the Phenomena Index and Theory in the Techniques Index)

2, 7, 8, 9, 10, 12, 16, 18, 23, 24, 26, 30, 31, 32, 34, 37, 50, 51, 52, 53, 54, 56, 58, 76, 80, 88, 95, 99, 112, 114, 121, 123, 129, 130, 132, 133, 145, 154, 156, 162, 170, 171, 181, 184, 185, 186, 190, 191, 192, 196, 198, 210, 218, 227, 240, 268, 269, 282, 283, 285, 308, 310, 317, 323, 329, 332, 342, 349, 362, 383, 385, 389, 407, 417, 420, 423, 434
(5.49, 3.76, 17.38)

Superconductors - metallic (also see superconductivity in the Phenomena Index and Theory in the Techniques Index)

12, 16, 30, 34, 50, 95, 130, 162, 181, 184, 185, 192, 229, 317, 406, 417
(1.13, 0.78, 3.61)

Superconductors - polymeric, organic (also see superconductivity in the Phenomena Index and Theory in the Techniques Index)

35
(0.07, 0.17, 0.23)

Semiconductor Materials - Elemental (including doped and amorphous phases)

15, 33, 56, 70, 71, 75, 89, 91, 93, 104, 108, 109, 114, 119, 122, 127, 130, 131, 139, 141, 146, 150, 169, 186, 190, 191, 194, 195, 211, 212, 217, 221, 222, 241, 250, 259, 260, 272, 284, 288, 291, 297, 325, 341, 346, 353, 367, 369, 375, 379, 409
(4.13, 2.36, 11.51)

## TECHNIQUES

Computer Simulation

3, 6, 18, 29, 33, 36, 37, 39, 56, 63, 64, 65, 67, 75, 89, 114, 116, 119, 122, 129, 130, 137, 144, 147, 149, 152, 156, 157, 160, 164, 165, 169, 171, 174, 175, 189, 197, 199, 204, 206, 210, 217, 219, 223, 224, 225, 242, 243, 244, 249, 253, 255, 266, 269, 272, 273, 287, 288, 306, 307, 309, 311, 322, 324, 325, 332, 363, 366, 377, 382, 388, 395, 398, 412, 421, 424, 426, 443
(3.97, 3.07, 17.61)

Chemical Vapor Deposition (all types)

31, 75, 76, 89, 94, 104, 106, 108, 109, 119, 141, 168, 186, 212, 213, 216, 217, 288, 353, 354, 404, 405, 427, 437
(1.11, 0.36, 5.42)

Dielectric Relaxation

182, 183, 266, 301, 303
(0.18, 0.07, 1.13)

Deep Level Transient Spectroscopy

119, 129, 141, 186, 323, 333, 354
(0.18, 0.10, 1.58)

Electron Diffraction (Technique development, not usage, for all types--LEED, RHEED, etc.)

14, 21, 22, 69, 75, 77, 79, 80, 89, 110, 111, 115, 116, 122, 138, 144, 154, 170, 172, 189, 195, 219, 226, 237, 240, 272, 300, 305, 311, 383, 394, 396, 405, 427, 430, 431
(1.47, 1.01, 8.13)

Electron Energy Loss Spectroscopy (EELS)

15, 21, 22, 30, 69, 70, 73, 75, 79, 80, 104, 110, 111, 114, 115, 116, 119, 144, 170, 172, 195, 215, 225, 226, 236, 237, 272, 296, 299, 300, 305, 372, 391, 430
(1.87, 1.03, 7.67)

Elastic Constants

23, 29, 156, 157, 170, 301, 355
(0.23, 0.16, 1.58)

Electrochemical Methods

21, 35, 36, 38, 49, 55, 60, 66, 79, 103, 131, 136, 137, 140, 141, 143, 182, 183, 196, 203, 205, 214, 266, 299, 302, 307, 357, 360, 368, 371, 403, 426
(1.58, 1.09, 7.22)

Electron Microscopy (technique development for all types)

1, 2, 3, 7, 22, 24, 34, 48, 69, 70, 75, 76, 80, 81, 89, 91, 107, 110, 111, 114, 115, 116, 117, 119, 132, 141, 148, 149, 152, 153, 154, 155, 157, 166, 168, 170, 172, 175, 176, 177, 178, 183, 186, 191, 206, 219, 225, 226, 240, 242, 254, 263, 272, 278, 279, 295, 299, 300, 308, 310, 311, 340, 341, 342, 348, 349, 360, 380, 404, 412, 414, 418, 436, 438
(5.15, 3.06, 16.70)

Electron Spectroscopy for Chemical Analysis (ESCA)

29, 31, 39, 58, 73, 76, 77, 79, 81, 104, 108, 118, 122, 139, 141, 144, 154, 157, 183, 263
(0.65, 0.43, 4.51)

Electron Spin Resonance or Electron Paramagnetic Resonance

37, 87, 119, 123, 166, 184, 214, 216, 266, 276, 315, 361
(0.50, 0.41, 2.71)

Extended X-Ray Absorption Fine Structure (EXAFS and XANES)

31, 32, 48, 49, 60, 76, 86, 131, 139, 150, 154, 222, 228, 263, 268, 284, 340, 344, 408, 409, 410, 423, 424, 425
(1.20, 0.76, 5.42)

Field Emission and Field Ion Microscopy

21, 24, 71, 170, 172, 209, 215, 341
(0.41, 0.32, 1.81)

High Pressure (Technique development of all types)

11, 28, 38, 129, 132, 159, 160, 162, 166, 197, 216, 252, 434
(0.68, 0.41, 2.93)

Ion or Molecular Beams

22, 37, 39, 40, 67, 77, 96, 107, 108, 119, 142, 162, 168, 170, 175, 186, 192, 193, 217, 230, 241, 250, 283
(1.06, 0.74, 5.19)

Ion Channeling, or Ion Scattering (including Rutherford and other ion scattering methods)

22, 25, 27, 39, 67, 70, 81, 107, 119, 146, 152, 170, 175, 183, 184, 193, 194, 211, 227, 241, 242, 311, 398
(1.15, 1.36, 5.19)

Internal Friction (also see Ultrasonic Testing and Wave Propagtion)

156, 266, 273
(0.09, 0.03, 0.68)

Infrared Spectroscopy (also see Raman Spectroscopy)

37, 38, 87, 124, 127, 132, 144, 160, 166, 182, 183, 186, 204, 210, 211, 218, 221, 224, 263, 266, 289, 301, 309, 333, 400
(1.22, 0.65, 5.64)

Laser Spectroscopy (scattering and diagnostics)

39, 40, 126, 127, 129, 135, 137, 138, 141, 151, 160, 168, 186, 197, 202, 206, 207, 212, 213, 217, 218, 221, 258, 290, 330, 334, 338, 364, 368, 381, 396, 411, 415, 428
(2.10, 0.72, 7.67)

Magnetic Susceptibility

5, 11, 12, 23, 29, 30, 35, 51, 116, 123, 132, 145, 152, 159, 162, 163, 185, 192, 214, 216, 259, 282, 285, 315, 361, 380, 407
(1.69, 1.00, 6.09)

Molecular Beam Epitaxy

29, 75, 77, 93, 94, 96, 107, 108, 109, 119, 138, 141, 168, 212, 213, 227, 240, 247, 284, 288, 409
(0.99, 0.34, 4.74)

Mossbauer Spectroscopy

30, 37, 116, 190, 248, 331, 390, 423, 425
(0.72, 0.22, 2.03)

Theory: Non-Destructive Evaluation



Theory: Surface



Theory: Structural Behavior



Theory: Superconductivity



Theory: Thermodynamics, Statistical Mechanics, and Critical Phenomena



Theory: Transport, Kinetics, Diffusion



Thermal Conductivity



Ultrasonic Testing and Wave Propagation



Vacuum Ultraviolet Spectroscopy



Work Functions

X-Ray Scattering and Diffraction (wide angle crystallography)

7, 13, 19, 23, 24, 29, 31, 32, 34, 35, 54, 55, 60, 63, 78, 86, 98, 116, 118, 119, 125, 135, 136, 139, 141, 145, 150, 152, 154, 156, 157, 160, 165, 166, 168, 171, 174, 190, 199, 206, 227, 240, 241, 249, 252, 261, 270, 274, 276, 277, 278, 280, 294, 309, 316, 327, 333, 337, 340, 349, 352, 354, 355, 370, 376, 407, 408, 410, 413, 426
(3.34, 1.70, 15.80)

X-Ray Scattering (small angle)

24, 29, 86, 116, 131, 139, 165, 171, 188, 210, 220, 222, 293, 295, 321, 352, 408, 411
(0.77, 0.73, 4.06)

X-Ray Scattering (other than crystallography)

13, 28, 32, 38, 41, 46, 49, 52, 55, 78, 116, 131, 141, 171, 174, 199, 222, 261, 262, 268, 284, 331, 358, 387, 390, 409, 436, 442
(1.58, 1.81, 6.32)

X-Ray Photoelectron Spectroscopy

19, 23, 37, 38, 39, 41, 46, 48, 58, 60, 72, 73, 104, 119, 122, 131, 138, 139, 141, 144, 146, 150, 161, 195, 203, 204, 209, 210, 222, 305, 319, 323, 398, 408
(1.40, 1.75, 7.67)

## PHENOMENA

Catalysis

21, 28, 37, 58, 79, 99, 122, 130, 134, 135, 138, 144, 188, 194, 195, 196, 197, 222, 226, 287, 296, 299, 344, 346, 387
(1.42, 1.36, 5.64)

Channeling

2, 56, 67, 70, 119, 175, 189, 194, 211, 227
(0.52, 0.41, 2.26)

Coatings (also see Surface Phenomena in this index)

21, 27, 40, 72, 104, 116, 130, 131, 134, 136, 138, 207, 245, 246, 268, 272, 353, 355, 398, 405, 434, 435
(1.31, 0.86, 4.97)

Colloidal Suspensions

87, 90, 118, 139, 154, 176, 179, 202, 210, 314, 364, 386
(0.81, 0.48, 2.71)

Conduction: Electronic

23, 35, 36, 60, 92, 96, 97, 99, 100, 101, 103, 119, 132, 137, 141, 166, 173, 185, 213, 214, 224, 227, 239, 242, 244, 259, 260, 275, 277, 289, 307, 308, 309, 330, 333, 345, 349, 354, 359, 362, 379, 384, 407, 412, 415
(2.75, 1.01, 10.16)

Conduction: Ionic

23, 36, 60, 92, 97, 100, 101, 137, 182, 183, 224, 266, 286, 303, 309, 333, 357
(1.13, 0.40, 3.84)

Dynamic Phenomena

33, 52, 107, 123, 126, 129, 137, 163, 180, 181, 189, 199, 208, 221, 237, 245, 283, 287, 290, 301, 324, 331, 381, 386, 387, 390, 396, 411, 415, 430, 439
(1.94, 0.89, 7.00)

Electronic Structure - Metals including amorphous forms

14, 18, 19, 30, 32, 56, 58, 93, 99, 109, 114, 130, 132, 137, 140, 149, 159, 161, 162, 164, 169, 173, 189, 219, 220, 222, 249, 265, 280, 281, 286, 323, 332, 337, 344, 359, 362, 367, 379, 384, 410, 420, 427
(2.03, 1.39, 9.71)

Electronic Structure - Non-metals including amorphous forms

18, 23, 31, 56, 76, 77, 93, 96, 103, 109, 126, 130, 137, 141, 146, 151, 162, 164, 166, 168, 169, 204, 221, 229, 244, 259, 260, 268, 285, 290, 329, 330, 332, 342, 354, 363, 366, 367, 375, 407, 415, 422
(3.05, 0.79, 9.48)

Erosion

343
(0.00, 0.00, 0.23)

Grain Boundaries

1, 3, 7, 24, 34, 48, 49, 51, 64, 65, 75, 81, 88, 114, 118, 119, 149, 155, 157, 164, 170, 172, 173, 175, 178, 190, 191, 203, 205, 219, 225, 235, 238, 242, 250, 271, 273, 278, 279, 280, 300, 306, 308, 318, 320, 322, 325, 337, 342, 348, 352, 356, 360, 372, 375, 378, 387, 401, 402, 404, 413, 431
(3.00, 1.68, 14.00)

Hydrogen Attack

80, 81, 160, 211, 230, 320, 360
(0.38, 0.17, 1.58)

Ion Beam Mixing

22, 25, 27, 39, 67, 108, 119, 193, 194, 196, 234, 250
(0.74, 1.22, 2.71)

Laser Radiation Heating (annealing, solidification, surface treatement)

39, 66, 77, 151, 153, 160, 161, 186, 190, 193, 194, 211, 287, 291, 347, 396, 439
(1.13, 0.87, 3.84)

Magnetism

1, 2, 5, 6, 7, 10, 11, 12, 18, 30, 32, 52, 53, 55, 58, 92, 109, 116, 122, 123, 133, 162, 173, 180, 185, 189, 220, 239, 244, 247, 254, 259, 261, 276, 277, 280, 282, 285, 315, 337, 359, 361, 362, 380, 383, 384, 394, 395, 417, 427
(2.82, 1.55, 11.29)

Martensitic Transformations and Transformation Toughening

4, 10, 13, 23, 53, 116, 148, 180, 267, 269, 301, 351
(0.52, 0.38, 2.71)

Mechanical Properties and Behavior: Constitutive Equations

84, 116, 135, 155, 157, 235, 343, 351, 378, 392
(0.34, 0.15, 2.26)

Mechanical Properties and Behavior: Creep

83, 84, 85, 116, 118, 160, 175, 176, 233, 235, 264, 319, 352, 401, 402, 413, 431
(0.59, 0.26, 3.84)

Mechanical Properties and Behavior: Fatigue

6, 83, 84, 85, 116, 118, 175, 231, 298, 302, 321, 326, 378, 392, 397
(0.61, 0.22, 3.39)

Mechanical Properties and Behavior: Flow Stress

3, 6, 84, 116, 155, 157, 160, 172, 242, 279, 326, 351, 404
(0.34, 0.19, 2.93)

Mechanical Properties and Behavior: Fracture and Fracture Toughness

3, 6, 23, 26, 83, 84, 85, 116, 118, 153, 154, 155, 157, 160, 175, 176, 178, 231, 235, 257, 278, 316, 317, 319, 321, 326, 339, 340, 343, 351, 370, 378, 395, 397, 402, 404, 413, 414, 421, 437
(2.01, 0.74, 9.03)

Materials Preparation and Characterization: Ceramics

19, 26, 31, 50, 54, 80, 88, 114, 118, 120, 132, 141, 153, 154, 155, 157, 162, 170, 172, 176, 182, 183, 188, 192, 196, 197, 202, 204, 207, 210, 218, 224, 242, 257, 263, 273, 290, 297, 300, 305, 308, 309, 319, 325, 333, 342, 350, 354, 370, 374, 385, 386, 392, 402, 404, 405, 413, 414, 440
(3.16, 1.55, 13.32)

Materials Preparation and Characterization: Glasses

32, 114, 154, 156, 182, 183, 184, 204, 210, 224, 232, 392
(0.47, 0.38, 2.71)

Materials Preparation and Characterization: Metals

1, 2, 8, 12, 13, 19, 22, 34, 39, 67, 114, 116, 117, 136, 137, 140, 141, 143, 144, 145, 148, 149, 157, 160, 161, 170, 172, 178, 184, 188, 227, 232, 240, 254, 255, 279, 280, 293, 298, 337, 339, 352, 360, 395, 404, 432, 433
(2.30, 1.45, 10.61)

Materials Preparation and Characterization: Polymers

60, 92, 97, 100, 101, 134, 135, 165, 183, 199, 202, 207, 295, 321, 335, 358, 407, 411, 415
(0.93, 0.44, 4.29)

Materials Preparation and Characterization: Semiconductors

13, 15, 56, 75, 93, 114, 119, 139, 141, 145, 166, 168, 212, 213, 232, 241, 284, 330, 353, 354, 409, 412, 426
(1.44, 0.55, 5.19)

Nondestructive Testing and Evaluation

3, 6, 144, 232, 298, 312, 443
(0.52, 0.14, 1.58)

Phonons

4, 10, 12, 18, 52, 102, 126, 127, 129, 130, 148, 151, 166, 168, 180, 181, 189, 218, 221, 232, 237, 239, 267, 269, 283, 296, 301, 376, 379, 391, 406, 415, 430
(1.83, 0.86, 7.45)

## ENVIRONMENT

## MAJOR FACILITIES: OPERATIONS