DOE/ER-0612P

February 1994

# Materials Sciences Programs

## Fiscal Year 1993

U.S. Department of Energy

Office of Energy Research

Office of Basic Energy Sciences

Division of Materials Sciences

DOE/ER-0612P
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February 1994

# Materials Sciences Programs
## Fiscal Year 1993

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 behavior 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 1993 together with a convenient index to the Division's programs. Recent publications from Division-sponsored panel meetings and workshops are listed on the following pages ii through v.

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 14 years. The contributions to them consist of scientists drawn from universities, national laboratories, and private sector industry, and represent a diverse mixture as well as a balance of sub-disciplines within materials science. It is our intention to make as much as possible of the proceedings of these activities publicly 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.

"Needed: Verified Models to Predict the Fracture of Weldments," D. W. Keefer, W. G. Reuter, J. A. Johnson, and S. A. David, Welding Journal, 72, 9, 1993, pp 73-79

"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, pp 1-246, 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, Mat. Sci. and Eng. A159 (1992), pp 1-34

"Deformation and Fracture of Intermetallics," M. H. Yoo, S. L. Sass, C. L. Fu, M. J. Mills, D. M. Dimiduk, E. P. George, Acta Metallurgica et Materialia, 41, 4, pp 987-1002, 1993

"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, Materials Science and Engineering, B18, 1993, pp 52-71

"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 1993 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 more detailed 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 provides cross-cutting 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 1993 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.

## DIVISION OF MATERIALS SCIENCES
Iran L. Thomas, Director, ER-13

Environment, Safety and Health, ER-13

Albert E. Evans
Michael F. Teresinski

Metallurgy and Ceramics Branch, ER-131

| Name | Program Area |
| --- | --- |
| Robert J. Gottschall | Electron Beam Microcharacterization Facilities |
| * Joseph B. Darby, Jr. | Physical Metallurgy |
| Alan L. Dragoo | Ceramics |
| Otto Buck | Mechanical Behavior, NDE |
| John N. Mundy | Physical Behavior, Irradiation Effects |
| Yok Chen | Physical Behavior, Irradiation Effects |
| Michael E. Kassner | Mechanical Behavior |
| Helen M. Kerch | Microstructure, Processing |

Solid State Physics and Materials Chemistry Branch, ER-132

| Name | Program Area |
| --- | --- |
| William T. Oosterhuis | Neutron and X-ray Facilities |
| Richard D. Kelley | Materials Chemistry, Polymers, Surface Science |
| Jerry J. Smith | Solid State Physics, Surface Science |
| Manfred Leiser | Solid State Theory |
| Harold L. Davis | Solid State and Surface Theory |
| Douglas K. Finnemore | Solid State Physics, Superconductivity, Magnetism |

* Retired as of December 30, 1993

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O. Buck 1/
J. N. Mundy 2/
Y. Chen 3/
M. E. Kassner 4/
H. M. Kerch 5/
J. B. Darby 8/

**Solid State Physics and Materials Chemistry Branch**

Chief: W. T. Oosterhuis

(Sharon A. Bowser-Secretary)

(301) 903-3426

R. D. Kelley
J. J. Smith
M. Leiser
H. L. Davis 6/
D. K. Finnemore7/

1/ On assignment from Ames Laboratory
2/ On assignment from Argonne National Laboratory
3/ On quarter-time assignment from Oak Ridge National Laboratory
4/ On quarter-time assignment from Oregon State University
5/ Interngovernmental Personnel Act assignee from Johns Hopkins University
6/ On part-time assignment from Oak Ridge National Laboratory
7/ On assignment from Ames Laboratory
8/ Retired as of December 30, 1993

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**SECTION E - OTHER USER FACILITIES**



**SECTION F - FUNDING LEVELS**

## SECTION G - INDEX

# SECTION A

Laboratories

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

## AMES LABORATORY

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

R. B. Thompson - (515) 294-9649
Fax: (515) 294-4456

### Metallurgy and Ceramics - 01

O. Buck - (515) 294-4446
Fax: (515) 294-8727

1. **SOLIDIFICATION MICROSTRUCTURES**
R. K. Trivedi, L. S. Chumbley, R. W. McCallum, J. D. Verhoeven
(515) 294-5869 01-1 $751,000

Studies of solidification processes and their applications to technologically important materials. Theoretical modeling of microstructural evolution and correlation between microstructures and processing conditions. Rapid solidification processing by the laser treatment of materials and by highly undercooled fine droplets. Development of microstructure/processing maps. Study of interface kinetics and the effect of crystalline anisotropy on the microstructure evolution. Directional solidification in organic materials such as succinonitrile, pivalic acid, carbontetrabromide, hexachleotyhane, t-butanol and naphthalene. 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, I. E. Anderson
(515) 294-9471 01-1 $312,000

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, O. Unal
(515) 294-4446 01-2 $456,000

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. 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 $130,650

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. Modeling pseudoelastic and thermoelastic behaviors of shape-memory alloys. 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 $340,000

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. **IRRADIATION INDUCED EMBRITTLEMENT IN METALS**
J. Kameda
(515) 294-7231 01-4 $146,000

Studies of segregation and desegregation of solutes at grain boundaries during neutron irradiation and post-irradiation annealing. Evaluation of mechanical properties including stress corrosion, hardening and embrittlement.

7. **ADVANCED MATERIALS AND PROCESSES**
I. E. Anderson, L. L. Jones, T. A. Lograsso, D. J. Sordelet
(515) 294-8252 01-5 $755,000

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. High pressure gas atomization for production of fine powders of metals and mixed metal oxides. Specialized coatings by plasma-arc spraying. Above research supported directly by the Materials Preparation Center described in the Section-Collaborative Research Centers.

8. **NDE MEASUREMENT TECHNIQUES**
O. Buck, D. C. Jiles, R. B. Thompson
(515) 294-4446 01-5 $254,000

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.

9. **SCIENTIFIC AND TECHNOLOGICAL INFORMATION EXCHANGE**
L. L. Jones, T. A. Lograsso, S. Mitra
(515) 294-5236 01-5 $186,000

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.

10. **FUNDAMENTALS OF PROCESSING OF BULK HIGH-$T_c$ SUPERCONDUCTORS**
R. W. McCallum, J. R. Clem, D. K. Finnemore, D. C. Johnson, M. J. Kramer
(515) 294-4736 01-5 $802,000

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.

**Solid State Physics - 02**

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

11. **NEUTRON SCATTERING**
C. Stassis, A. Goldman, D. Vaknin, J. Zarestky
(515) 294-4224 02-1 $430,950

Study of the magnetic properties of high temperature superconductors and related compounds by polarized and unpolarized neutron scattering techniques ($La_2CuO_4$, $LaNiO_4$, $La_{2-x}Sr_xCuO_4$, $La_{2-x}Sr_xNiO_4$). Experimental investigation of the lattice dynamics of metals and alloys undergoing martensitic transformations (bcc La, Cu-Al-Be, Cu-Al-Ni, Cu-Zn-Al); study of the Verwey transition in magnetite. Electronic structure and phonon spectra of mixed valence compounds ($CePd_3$, $_\gamma$-Ce). Lattice dynamics of quasicrystals. Study of organized films on aqueous and solid surfaces by neutron and X-ray reflectivity techniques.

12. **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 $682,500

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 and/or competition 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.

13. **SUPERCONDUCTIVITY**
D. K. Finnemore, J. E. Ostenson
(515) 294-3455 02-2 $273,000

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

14. **X-RAY DIFFRACTION PHYSICS**
A. Goldman
(515) 294-3585 02-2 $243,750

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 and spectroscopy. Development of beamlines at APS.

15. **OPTICAL, SPECTROSCOPIC, AND SURFACE PROPERTIES OF SOLIDS**
D. W. Lynch, C. G. Olson, M. Tringides
(515) 294-3476 02-2 $619,125

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. Epitaxial growth on metal and semiconductor surfaces, surface diffusion, ultrathin film morphology, LEED (Low Energy Electron Diffraction), RHEED (Reflection, High Energy Electron Diffraction), STM (Scanning Tunneling Microscopy) are used for structural characterization and time dependent measurements. Vacuum microelectronics studies of field emission arrays for flat panel displays.

16. **SEMICONDUCTOR PHYSICS**
J. Shinar
(515) 294-8706 02-2 $243,750

(i) Fabrication and electronic and structural dynamics studies of hydrogenated amorphous Si-based thin films and devices, using UV-Vis-NIR-IR absorption spectroscopies, photoconductivity, SAXS, and SIMS. (ii) Processing and studies of fullerenes, using luminescence and optically-detected magnetic resonance spectroscopies. (iii) Fabrication and characterization of thin diamond and porous Si films and devices.

17. **SUPERCONDUCTIVITY THEORY**
J. R. Clem, V. Kogan
(515) 294-4223 02-3 $146,250

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, proximity effects, and vortex fluctuations.

18. **OPTICAL AND SURFACE PHYSICS THEORY**
R. Fuchs, C. T. Chan, K.-M. Ho
(515) 294-1960 02-3 $146,250

Optical properties of metals, semiconductors, and insulators, studies of surfaces, thin films, layered systems, small particles, and powders. Differential surface reflectance spectroscopy. Photonic band structure. Electron energy-loss spectroscopy of inhomogeneous systems. First principles calculation of lattice relaxation, reconstruction and phonons at single crystal surfaces (Al, Au, W, Mo, Ag, and Au on Si). Chemisorption. Determination of growth modes via first principles calculations.

19. **ELECTRONIC AND MAGNETIC PROPERTIES**
B. N. Harmon, C. T. Chan, K.-M. Ho, M. Luban, C. Soukoulis
(515) 294-7712 02-3 $479,000

Theoretical studies of bulk and lattice dynamical properties of materials using first principles total energy calculations. Magnetic properties of new high-$T_c$ superconductors. 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 and Bloch oscillations. Buckyballs.

**Materials Chemistry - 03**

P. A. Thiel - (515) 294-8985
Fax: (515) 294-4709

20. **SYNTHESIS AND CHEMICAL STRUCTURE**
J. D. Corbett, J. W. Anderegg, H. F. Franzen, R. A. Jacobson, R. E. McCarley
(515) 296-3086 03-1 $741,000

Synthesis and structure of and bonding in polar intermetallic 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 intermetallic 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.

21. **POLYMER AND ENGINEERING CHEMISTRY**
T. J. Barton, M. Akinc, S. Ijadi-Maghsoodi
(515) 294-2770 03-2 $464,000

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.

22. **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 $534,000

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, electrochemical incineration, 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. Equilibrium and dynamic properties of adsorbed films. 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

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**Metallurgy and Ceramics - 01**

B. D. Dunlap - (708) 252-4925
Fax: (708) 252-4798

23. **ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH**
N. J. Zaluzec, C. W. Allen
(708) 252-5075 01-1 $1,463,000

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 six months. A state-of-the-art, medium-voltage, ultra-high vacuum, field-emission gun, Analytical Electron Microscope is being installed. 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).

24. **INTERFACE STUDIES**
K. L. Merkle, J. N. Mundy
(708) 252-4990 01-3 $657,000

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. **BASIC CERAMICS**
B. W. Veal, S.-K. Chan, J. L. Routbort
(708) 252-4957 01-3 $1,197,000

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 photoelectron (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.

26. **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 $1,620,000

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. Studies of neutron irradiation effects on alloy microstructure. Irradiation performance of advanced nuclear fuels. Effects of amorphization on dimensional stability. Radiation-induced segregation to internal and external defect sinks. Radiation-enhanced diffusion. 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. 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.

27. **HIGH-$T_c$ SUPERCONDUCTOR DEVELOPMENT**
G. W. Crabtree, K. Goretta, J. L. Routbort, D. Shi
(708) 252-5509 01-5 $593,000

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.

**28. AMORPHOUS AND NANOCRYSTALLINE MATERIALS**
L. E. Rehn, J. Eastman, N. Q. Lam, P. R. Okamoto, R. W. Siegel
(708) 252-5021 01-5 $634,000

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.

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**Solid State Physics - 02**

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**29. NEUTRON AND X-RAY SCATTERING**
J. D. Jorgensen, J. E. Epperson, G. P. Felcher, R. Kleb, R. Osborn, D. L. Price
(708) 252-5513 02-1 $1,591,000

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.

**30. TWO-DIMENSIONAL MATERIALS**
S. D. Bader, M. B. Brodsky, M. Grimsditch
(708) 252-4960 02-2 $841,000

Research on the growth and physical properties of novel ultra-thin, epitaxial films, metallic sandwiches, superlattices and multilayers. Thin-film and surface-science preparation techniques include molecular beam epitaxy, 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 (photoemission and Auger), band-structure theory, and low-temperature transport, magnetic and magneto-optic Kerr effect measurements. Elastic, magnetic and vibrational properties using Brillouin and Raman scattering, and spin polarized photoemission.

**31. 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 $1,333,000

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.

**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 $538,000

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 beamline 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. **CERAMIC EPITAXY AND MULTILAYER STRUCTURES**
B. W. Veal, H. L. Chang
(708) 252-4957 02-2 $430,000

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: $TiO_2$, $VO_2$, $BaTiO_3$, $PbTiO_3$, $PbZrO_3$, 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.

34. **CONDENSED MATTER THEORY**
A. A. Abrikosov, R. Benedek, R. A. Klemm, D. D. Koelling, M. Norman, M. Randeria, N. Trivedi
(708) 252-5482 02-3 $1,124,000

Theory of superconductivity; electronic band structure, many-body effects; properties of low-dimensional systems. Physical properties of layered superconductors including anisotropic energy gap. Vortex lattice. Superconductivity in heavy-fermion and high-$T_c$ materials. Reentrant superconductivity in strong magnetic fields. Organic superconductors. Contributions of fluctuations superconductor-insulator transition. Normal state anomalies in high-$T_c$ superconductors. Strongly correlated systems. Quantum Monte Carlo methods. Electronic band structure calculations of narrow band systems. Correlation effects in metals and metal oxides. Large cell computational methods and their applications for cohesive properties. Intercalated layered substances. Multilayered materials. Anderson localization in quasi 1- and 2-dimensional metals. Disordered boron systems.

35. **MODELING AND THEORY OF INTERFACES**
D. Wolf, S. Phillpot, S. Yip
(708) 252-5205 02-3 $258,000

Computer simulation of the physical properties of solid interfaces, such as grain and interphase boundaries, free surfaces thin films, nanocomposites 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 grain and phase boundaries as a function of temperature, the dielectric behavior of surfaces and grain boundaries in perovskite materials, and the properties of steps in free surfaces. Materials considered involve metals, semiconductors and predominantly ionic ceramics as well as interfaces between them.

36. **ULTRA-HIGH FIELD SUPERCONDUCTORS**
K. E. Gray, R. T. Kampwirth, D. J. Miller
(708) 252-5525 02-5 $360,000

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.

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**Materials Chemistry - 03**

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37. **CHEMICAL AND ELECTRONIC STRUCTURE**
J. M. Williams, K. D. Carlson, U. Geiser, A. M. Kini, J. S. Schlueter, J. Schultz
(708) 252-3464 03-1 $1,329,000

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) by use of the IPNS-SCD and a low-temperature (10 K) single crystal X-ray diffraction instrument.

38. **THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS**
M. Blander, L. A. Curtiss, M.-L. Saboungi
(708) 252-4548 03-2 $500,000

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.

39. **INTERFACIAL MATERIALS CHEMISTRY**
V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, A. R. Krauss
(708) 252-4547 03-2 $491,000

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 orbital calculations of chemical properties of zeolite catalysts 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.

40. **AQUEOUS CORROSION**
V. A. Maroni, L. A. Curtiss, C. A. Melendres, Z. Nagy, R. M. Yonco
(708) 252-4547 03-2 $628,000

Basic research aimed at elucidating fundamental aspects of interfacial phenomena that occur under conditions of temperature and pressure (300°C and 10 MPa) relevant to light water fission reactors, 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, photoelectrochemical and X-ray methods. 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. Theoretical/computational simulations of solid\liquid interface phenomena through the application of molecular dynamics methods in combination with ab initio molecular orbital theory.

41. **PARTICLE AND PHOTON INTERACTIONS WITH SURFACES**
D. M. Gruen, W. F. Calaway, A. R. Krauss, G. J. Lamich, M. J. Pellin
(708) 252-3513 03-3 $1,002,000

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.

42. **MOLECULAR IDENTIFICATION FOR SURFACE ANALYSIS**
D. M. Gruen, K. R. Lykke, M. J. Pellin
(708) 252-3513 03-3 $422,000

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**

43. **APS USER TECHNICAL AND ADMINISTRATIVE INTERFACE**
S. Barr, S. Davey, G. K. Shenoy
(708) 252-5537 04-1 $663,000

The user technical and administrative interface will provide the point of contact between the APS and the APS users during the design, construction, and operation of users' experimental beamlines. This program will provide for the integration of user technical and administrative requirements with APS Experimental Facilities Division activities and for the oversight and support during development of these beamlines.

44. **APS ACCELERATOR R&D**
M. Borland, E. Crosbie, R. Damm, G. Decker, H. Friedsam, J. Galayda, G. Goeppner, R. Kustom, A. Lumpkin, G. Mavrogenes, D. McGhee, F. Mills, S. Milton, J. Noonan, S. Sharma, L. Teng, M. White
(708) 252-7796 04-1 $7,456,000

This research supports construction of the Advanced Photon Source, 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 of the accelerator and storage ring systems. Theoretical methods are developed and applied to predict accelerator physics performance parameters. Facility Title II design activities began in FY 1990, construction was initiated in FY 1990 and completion is scheduled for FY 1997.

45. **INTENSE PULSED NEUTRON SOURCE PROGRAM**
B. S. Brown, F. R. Brumwell, J. M. Carpenter, W. D. Ruzicker
(708) 252-4999 04-1 $6,644,000

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 250 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.

46. **APS COMMISSIONING AND START-UP**
Y. Cho, J. Galayda, G. Shenoy
(708) 252-6616 04-1 $10,553,000

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 correctly. 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.

47. **ASD R&D IN SUPPORT OF OPERATIONS**
E. Crosbie, R. Damm, J. Galayda, M. Knott, R. Kustom, A. Lumpkin, G. Mavrogenes, L. Teng, M. White
(708) 252-7796 04-1 $6,652,000

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 linesto 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.

48. **APS BEAMLINE AND INSERTION DEVICE R&D**
E. Gluskin, T. Kuzay, D. M. Mills, G. K. Shenoy
(708) 252-5537 04-1 $11,988,000

Experimental Facilities R&D supports the construction of various APS components such as the insertion devices, mechanical components of the beamline front ends and transport, X-ray optics, detectors, and synchrotron instruments. This R&D, including the construction and testing of prototypes, is needed to assure that the detailed designs meet or exceed the desired performance goals of the APS construction project and to assure that the APS user community can perform their research.

49. **XFD R&D IN SUPPORT OF OPERATIONS**
E. Gluskin, D. M. Mills, G. K. Shenoy
(708) 252-5537 04-1 $4,335,000

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 instrumentation. 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.

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**Metallurgy and Ceramics - 01**

K. G. Lynn - (516) 282-3501
Fax: (516) 282-4071

50. **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 $458,000

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. Electronic structure.

51. **STRUCTURE AND PROPERTIES OF SURFACE MODIFIED MATERIALS AND INTERFACES**
S. M. Heald, B. Nielsen
(516) 282-2861 01-1 $493,000

Experimental studies of the fundamental factors which influence the microstructure and chemical bonding at interfaces between dissimilar materials and of thin films of materials which have been modified by various means to have properties different from those within the bulk of the materials (metals, semiconductors, insulators). 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.

52. **MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS**
H. S. Isaacs, A. J. Davenport
(516) 282-4516 01-2 $557,000

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. Concentrations and valency of elements in surface oxides using X-ray absorption. Studies of the role of corrosion-inhibitors and the mobility of inhibiting anions under existing high electric fields. 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 simulating localized corrosion. Structure of the electrolytes, salt film formation, and electromigration.

53. **SUPERCONDUCTING MATERIALS**
M. Suenaga, R. Budhani, D. O. Welch, Y. Zhu
(516) 282-3517 01-3 $1,139,000

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.

54. **BASIC MATERIALS SCIENCE OF HIGH-$T_c$ CONDUCTOR FABRICATION**
M. Suenaga, Q. Li, Y. Zhu
(516) 282-3518 01-5 $608,000

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 $Bi_2Sr_2Ca_2Cu_3O_8$ 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 $YBa_2Cu_3O_7$ and $Bi_2Sr_2Ca_2Cu_3O_8$ to strengthen the coupling of the boundaries by various methods.

**Solid State Physics - 02**

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55. **ELEMENTARY EXCITATIONS AND NEW TECHNIQUES**
S. M. Shapiro, L. Passell, B. Sternlieb, T. Thurston, L. Ye
(516) 282-3822 02-1 $1,398,000

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.

56. **MAGNETIC AND STRUCTURAL PHASE TRANSITIONS**
J. M. Tranquada, H. Chou, P. M. Gehring, K. Hirota, G. Shirane
(516) 282-3732 02-1 $1,143,000

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.

57. **STRUCTURAL CHARACTERIZATION OF MATERIALS USING POWDER DIFFRACTION TECHNIQUES**
D. E. Cox, J. A. Hriljac
(516) 282-3818 02-2 $283,000

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. 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.

58. **EXPERIMENTAL RESEARCH - X-RAY SCATTERING**
L. D. Gibbs, G. Helgesen, J. P. Hill, O. Magnussen, B. Ocko, T. Thurston, G. Watson
(516) 282-4608 02-2 $1,272,000

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 three participating research teams, operates and maintains three X-ray beamlines at the National Synchrotron Light Source (X22A, X22B, and X22C) and is involved in the development and use of two new insertion device beamlines (X21 and X25). Particular emphasis is placed on 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 metal surface phase transformations 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) X-ray magnetic scattering studies of bulk and thin film rare earths, transition elements, and actinides.

59. **LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS**
K. G. Lynn, P. Asoka-kumar, Y. Kong, P. Simpson
(516) 282-3710 02-2 $1,012,000

A new initiative using Ac-cross-correlational technique to understand the fundamental mechanism responsible for the 1/f noise was started. 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.

60. **THEORETICAL RESEARCH**
J. W. Davenport, P. Bak, V. J. Emery, M. Pacuski, R. E. Watson, M. Weinhert
(516) 282-3789 02-3 $860,000

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.

61. **SURFACE PHYSICS RESEARCH**
M. Strongin, P. D. Johnson, P. Koiper, M. W. Ruckman, K.-D. Tsuei
(516) 282-3763 02-5 $949,000

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 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 and electronic properties of metal overlayers; (d) surface metallurgy and surface compounds; and (e) studies of charge transfer and metastable species formed in low temperature reactions; and (f) formation of surface coating using cryogenic techniques and synchrotron radiation.

**Materials Chemistry - 03**

62. **NEUTRON SCATTERING - SYNTHESIS AND STRUCTURE**
J. Z. Larese
(516) 282-4349 03-1 $461,000

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 Multidetector 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 now available. Each of the new detectors provides more than an order of magnitude increase in data collection efficiency.

63. **SYNTHESIS AND STRUCTURES OF NEW CONDUCTING POLYMERS**
J. McBreen
(516) 282-4513 03-2 $475,000

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, Raman 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**

64. **EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS**
M. H. Brooks, W. Brynda, J. Detweiler, O. Jacobi, L. Junker, V. Lettieri, J. Petro, T. Prach, R. Reyer, D. C. Rorer, P. Tichler
(516) 282-4061 04-1 $23,233,000

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.

65. **NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT**
D. B. McWhan, N. Fewell, J. Hastings, R. Heese, J. Keane, R. Klaffky, S. Kramer, S. Krinsky, W. Thomlinson
(516) 282-3927 04-1 $16,491,000

This program supports the operation of the National Synchrotron Light Source, which is a large user facility devoted to the production and utilization of synchrotron radiation, and its supports the development of electron based radiation sources and of 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 improve 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. The PRTs continue to invest heavily in the facility, and the program seeks to keep the facility at the forefront to justify this investment. To do this, a six-year plan has been developed to improve the storage rings, to provide the needed complement of state-of-the-art beamlines and to provide needed user support.

## IDAHO NATIONAL ENGINEERING LABORATORY

**Idaho Falls, ID 83415**

D. W. Keefer - (208) 526-8003
Fax: (208) 526-0263

66. **STRESS DISTRIBUTION IN GRADED MICROSTRUCTURES**
B. H. Rabin
(208) 526-0058 01-5 $218,000

Develop fundamental understanding of the effects of microstructure, processing conditions, and specimen geometry on the thermomechanical behavior of graded materials for the purpose of mitigating the property mismatch at dissimilar material interfaces. Fabrication of two-phase coatings and bulk materials with controlled microstructural gradients and varying geometries by ion-beam assisted deposition (IBAD) and powder metallurgy techniques. Focus on model materials systems in which significant property mismatch exists between components, e.g., $AL_2O_3$/Ni. Mapping of residual stresses by high spatial resolution X-ray and neutron diffraction methods. Comparison of experimental results with predictions from elastic-plastic finite element method (FEM) modeling of stress distributions. Use of FEM models to design gradient material microstructures to meet application requirements.

67. **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 studies in simple systems to determine fundamental mechanisms. Initial studies of high-purity aluminum and aluminum doped with ppm levels of lead or indium containing ion-implanted helium have shown accelerated helium bubble growth when liquid precipitates are attached to bubbles. 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, have been examined. Experimental techniques include positron annihilation and TEM. The transformation from a dendritic as-solidified structure to equiaxed grains during isothermal annealing is being studied in detail for a Ag-2% Al alloy.

## UNIVERSITY OF ILLINOIS MRL

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**Urbana, IL 61801**

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Fax: (217) 244-2278

**Metallurgy and Ceramics - 01**

H. Birnbaum - (217) 333-1370
Fax: (217) 244-2278

68. **THEORY OF DEFECTS AND INTERFACES IN BCC METALS**
J. Adams
(217) 244-7709 01-1 $206,691

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.

69. **TRANSPORT PROCESSES IN LOCALIZED CORROSION**
R. C. Alkire
(217) 333-3640 01-1 $214,591

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

70. **DEFECTS, DIFFUSION, AND NON-EQUILIBRIUM PROCESSING OF MATERIALS**
R. S. Averback
(217) 333-4302 01-1 $323,728

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.

71. **MOLECULAR SPECTROSCOPY OF THE SOLID-LIQUID INTERFACE**
P. W. Bohn
(217) 333-0676 01-1 $84,662

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 adsorbate-substrate binding and linear dichroism to probe the supermolecular structure and molecular orientation. Correlation with the solution chemistry and corrosion response will be made.

72. **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.

73. **MICROANALYSIS OF DEFECTS AND INTERFACES**
J. A. Eades
(217) 333-8396 01-1 $164,031

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.

74. **ATOMISTICS OF GROWTH AND TRANSPORT AT METAL AND SEMICONDUCTOR INTERFACES**
G. Ehrlich
(217) 333-6448 01-1 $159,986

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.

75. **ATOMIC RESOLUTION ELECTROCHEMISTRY OF CORROSION AND DEPOSITION PROCESSES**
A. A. Gewirth
(217) 333-8329 01-1 $95,017

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

76. **TRANSMISSION ELECTRON MICROSCOPY OF SURFACES AND INTERFACES**
J. M. Gibson
(217) 333-2997 01-1 $208,571

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.

77. **CRYSTAL GROWTH AND PHYSICAL PROPERTIES OF METASTABLE SEMICONDUCTING, CERAMIC AND METALLIC ALLOYS**
J. E. Greene
(217) 333-0747 01-1 $197,889

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 II-IV-V2 chalcopyrite systems.

78. **SURFACE AND INTERFACE X-RAY DIFFRACTION**
I. K. Robinson
(217) 244-2949 01-1 $114,862

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 $176,231

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 $203,873

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 $184,282

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. **APPLICATION OF SURFACE CHEMISTRY TECHNIQUES TO UNDERSTANDING HETEROEPITAXY**
H. Farrell
(217) 333-0386 01-2 $70,121

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.

83. **COUNCIL ON MATERIALS SCIENCE**
C. P. Flynn
(217) 333-1370 01-2 $55,551

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.

84. **CHEMISTRY OF NEW TRANSITION METAL CERAMIC COMPOUNDS SYNTHESIZED BY MOCVD**
G. S. Girolami
(217) 333-2729 01-2 $76,143

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.

85. **HIGH TEMPERATURE MECHANICAL BEHAVIOR OF CERAMICS**
D. F. Socie
(217) 333-7630 01-2 $94,556

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.

86. **MICROSTRUCTURE BASED CONTINUUM MODELING OF THE MECHANICAL BEHAVIOR OF MATERIALS**
P. Sofronis
(217) 333-2636 01-2 $69,306

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.

87. **SUBCRITICAL CRACK GROWTH IN STRUCTURAL CERAMICS**
J. F. Stubbins
(217) 333-6474 01-2 $54,575

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.

88. **STRUCTURE AND KINETICS OF ORDERING TRANSFORMATIONS IN METAL ALLOYS AND SILICIDE THIN FILMS**
H. Chen
(217) 333-7636 01-3 $137,013

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.

89. **MATERIALS CHEMISTRY OF OXIDES CERAMICS; FIELD RESPONSIVE ORGANIC INCLUSION COMPLEXES**
W. F. Klemperer
(217) 333-2995 01-3 $216,381

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.

90. **SYNTHESIS AND PROPERTIES OF ELECTRICAL CERAMICS**
D. A. Payne
(217) 333-2937 01-3 $311,356

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.

91. **ATOMIC SCALE MECHANISMS OF VAPOR PHASE CRYSTAL GROWTH**
A. Rockett
(217) 333-0417 01-3 $140,416

Theoretical studies of the atomic scale processes which determine the surface structures of crystals during vapor phase growth. Monte Carlo emulations 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.

92. **MAGNETIC BEHAVIOR OF NANOPHASE MATERIALS**
M. B. Salamon
(217) 333-6186 01-3 $48,083

Experimental and theoretical studies of the magnetic properties of nanophase metals and mixtures of metals. Interfacial effects of magnetic particles embedded in non-magnetic matrices. Investigation of spin waves, quantum tunneling of the macroscopic magnetization of particles and macroscopic quantum coherence effects.

93. **PROCESSING OF MONODISPERSE CERAMIC POWDERS**
C. Zukoski
(217) 333-7379 01-3 $225,819

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.

94. **MICROSCOPIC PROCESSES IN IRRADIATED CRYSTALS**
R. S. Averback, C. P. Flynn
(217) 333-4302 01-4 $181,008

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.

95. **RADIATION EFFECTS IN METALS AND SEMICONDUCTORS**
I. M. Robertson
(217) 333-6776 01-4 $136,992

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
Fax: (217) 244-2278

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96. **SYNTHESIS AND CHARACTERIZATION OF ORGANOMETALLIC LIQUID CRYSTAL POLYMERS**
T. L. Brown
(217) 244-1176 02-2 $51,599

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

97. **MICROSCOPIC MECHANISMS OF CRYSTAL GROWTH**
D. Cahill
(217) 333-6753 02-2 $65,813

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.

98. **ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES**
T.-C. Chiang
(217) 333-2593 02-2 $160,538

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.

99. **OPTICAL AND MAGNETO-OPTICAL STUDIES OF THE ELECTRONIC STRUCTURE OF SOLIDS**
S. L. Cooper
(217) 333-2589 02-2 $51,340

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.

100. **GROWTH AND PROPERTIES OF NOVEL MBE MATERIALS**
C. P. Flynn
(217) 244-6297 02-2 $172,935

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.

101. **THEORY OF SOLIDS, SURFACES AND HETEROSTRUCTURES**
R. M. Martin
(217) 333-4229 02-3 $96,299

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.

102. **SEMICONDUCTOR/INSULATOR STRUCTURES**
H. Morkoc
(217) 333-0722 02-2 $120,455

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.

103. **DESIGN AND SYNTHESIS OF NEW ORGANOMETALLIC MATERIALS**
T. B. Rauchfuss
(217) 333-7355 02-2 $117,675

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 vortices of metal clusters will be used to generate clusters-of-clusters. Synthetic studies will focus on charge transfer salts containing organometallic donors and acceptors.

104. **MICROSCOPIC THEORIES OF THE STRUCTURE AND PHASE TRANSITIONS OF POLYMERIC MATERIALS**
K. S. Schweizer
(217) 333-6440 02-2 $45,956

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.

105. **PROPERTIES OF CRYSTALLINE AND LIQUID CONDENSED GASES**
R. O. Simmons
(217) 333-4170 02-2 $170,274

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.

106. **NUCLEAR MAGNETIC RESONANCE IN SOLIDS**
C. P. Slichter
(217) 333-3834 02-2 $233,029

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.

107. **ELECTRO-ACTIVE AND NONLINEAR OPTICAL POLYMERS**
S. I. Stupp
(217) 333-4436 02-2 $207,523

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.

108. **METALLOPORPHYRINS AS FIELD RESPONSIVE MATERIALS**
K. S. Suslick
(217) 333-2794 02-2 $65,491

The synthesis and characterization of porphyritic materials with ferroelectric and nonlinear 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.

109. **CARRIER TRANSPORT IN QUANTUM WELLS - PICOSECOND IMAGING**
J. P. Wolfe
(217) 333-2374 02-2 $115,021

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.

**Materials Chemistry - 03**

T.-C. Chiang - (217) 333-2593
Fax: (217) 244-2278

110. **HIGH PRESSURE STUDIES OF MOLECULAR AND ELECTRONIC PHENOMENA**
H. G. Drickamer
(217) 333-0025 03-1 $184,797

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.

111. **MECHANISTIC AND SYNTHETIC STUDIES IN CHEMICAL VAPOR DEPOSITION**
R. G. Nuzzo
(217) 244-0809 03-1 $155,065

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.

112. **OPTICAL SPECTROSCOPY OF SURFACE PROCESSES IN THIN FILM DEPOSITION**
E. G. Seebauer
(217) 333-4402 03-3 $31,657

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**

113. **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, computer image analysis, simulation, and processing.

114. **CRYSTALLOGRAPHY OF MICROSTRUCTURES**
U. Dahmen
(510) 486-4627 01-1 $187,000

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 characterization of the atomic structure of interfaces by conventional, in situ and atomic resolution microscopy in tandem with computer image simulations.

115. **ALLOY PHASE STABILITY**
D. de Fontaine
(510) 486-8177 01-1 $200,000

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.

116. **IN SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY**
J. W. Evans
(510) 486-3807 01-1 $28,000

Microstructural aspects of gas-solid reactions. Focus of attention is porous silicon, its oxidation and densification of the oxide by viscous flow. Porous silicon is effective in reducing oxidation induced stacking faults in silicon wafer 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 densifies 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.

117. **STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES**
R. Gronsky
(510) 486-5674 01-1 $156,000

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.

118. **THIN FILM STRUCTURES AND COATINGS**
K. Krishnan
(510) 486-4614 01-1 $104,000

This program seeks to establish a dynamic iteration between forefront efforts in synthesis, experimental investigation of microstructures and property measurements with the goal of atomically engineering thin films with novel mechanical, optical and magnetic properties. Fundamental investigations of new phenomena and mechanisms influencing improved properties will be stressed. In addition to synthesis, development of nanoscale spectroscopy, 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 multilayers exhibiting either perpendicular anisotropy or long-range antiferromagnetic coupling, studies of the changes in electronic structure 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 of the films are also being addressed.

119. **CAM CERAMIC SCIENCE PROGRAM**
L. C. DeJonghe, R. Cannon, B. Dalgulsh, A. Glaeser, R. Ritchie, G. Thomas, A. Tomsia
(510) 486-6138 01-3 $1,423,000

The CAM Ceramic 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 performance beyond 1900 K, and the evaluation of the mechanical properties of these ceramics, at temperatures above 1700 K. 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 characterizes micro- and nano-chemistry and structure in relation to high temperature mechanical and environmental performance.

120. **CAM ELECTRONIC MATERIALS PROGRAM**
E. Haller, E. Bourret, Z. Lilental, W. Walukiewicz, J. Washburn, E Weber, K. M. Yu
(510) 486-5294 01-3 $1,181,000

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.

121. **HIGH-TEMPERATURE REACTIONS**
A. W. Searcy
(510) 486-5900 01-3 $35,000

Sintering studies of 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**

122. **QUANTUM SIZE EFFECTS IN SEMICONDUCTOR NANOSTRUCTURES**
D. S. Chemla
(510) 486-4999 02-2 $197,000

The objective of this program is to explore the physical properties of low dimensionality materials, i.e., material systems whose sizes are intermediate between that of atoms/molecules and that of bulk solids. Because of quantum mechanical size effects, the properties of such systems are size and shape dependent and neither like those of atoms or those of macroscopic solids. They open new avenues for unprecedented experiments testing the limits of our understanding of condensed matter physics (see for example DOE Council on Materials Science Panel Report, J. Mater. Res. Vol. 4 No 3,704, 1989). The research emphasizes the study of the nature and dynamics of electronic collective excitations in ultra-thin, quasi-2D layers, as well as the effects of dimensionality on the light-matter interaction. Unique time resolved-tunable ultrashort pulse laser spectroscopy techniques are specifically developed for these investigations. Recent work has focused on the dynamics of the instantaneous frequency and amplitude of coherent light scattering from quasi-2D excitons, and on the dimensionality dependence of the thermalization of electron-hole plasmas. The program will be extended to the further confinement of electronic states, into 1D and 0D, by application of high magnetic fields.

123. **SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE**
J. Clarke
(510) 642-3069 02-2 $211,000

DC Superconduct 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 1 MHz. Origins of low frequency magnetic noise, mechanisms of flux pinning and dissipation, 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.

124. **SURFACE, INTERFACE, AND NANOSTRUCTURE STUDIES USING SYNCHROTRON RADIATION IN COMBINATION WITH OTHER PROBES**
C. S. Fadley
(510) 486-5774 02-2 $246,000

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 semiconductors (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 and short-range magnetic order 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 has been completed.

125. **NONLINEAR EXCITATIONS IN SOLID-STATE SYSTEMS**
C. D. Jeffries
(510) 486-3382 02-2 $125,000

One area of study is nonlinear dynamics and instabilities in solid state systems. The objectives are detailed experimental studies of block wall jumps in amorphous ferromagnets spin wave instabilities in magnetic garnets. The observed behavior is compared to various theoretical models. Another area of study is high-temperature superconductivity using microwave and radio frequency 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.

126. **FAR-INFRARED SPECTROSCOPY**
P. L. Richards
(510) 486-3027 02-2 $194,000

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, 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.

127. **STUDIES OF THE METAL/SOLUTION INTERFACE WITH X-RAYS**
P. N. Ross
(510) 486-6226 02-2 $187,000

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.

128. **FEMTOSECOND DYNAMICS IN CONDENSED MATTER**
C. V. Shank
(510) 486-5111 02-2 $285,000

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 measurement 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 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 nanocrystals). Experimental results show clear evidence of coherent vibrational oscillations which modulate the dynamic dephasing of the optically excited electron-hole paris 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. Three-pulse photon echo measurements in CdSe indicate that electronic dephasing occurs on a 100 fs time scale at 15 K, with significant contributions from an acoustic phonon heatbath. Contributions from acoustic phonons dominate the dephasing at room temperature. Three-pulse photon echo techniques are being applied to studies of electronic dephasing of oxazine molecules in solution. Preliminary results indicated a dependence of the dephasing rate on the solvent environment. This will provide a foundation for studying solvent-solute interactions. In addition, we are applying femtosecond techniques to study electronic and vibrational dynamics in $C_{60}$. Relaxation processes in this material exhibit highly non-exponential behavior resulting from exciton-exciton annihilation process. We also observe coherent vibrational oscillations corresponding to breathing and pinching modes of the $C_{60}$ molecule. These studies of ultrafast processes in condensed matter will provide new information about the fundamental properties of materials. This knowledge will be useful for evaluating novel materials for future energy applications.

129. **EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS**
Y. R. Shen
(510) 486-4856 02-2 $221,000

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.

130. **TIME-RESOLVED SPECTROSCOPIES IN SOLIDS**
P. Y. Yu
(510) 486-8087 02-2 $135,000

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.

131. **QUANTUM THEORY OF MATERIALS**
M. L. Cohen, L. M. Falicov, S. G. Louie
(510) 486-4753 02-3 $402,000

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. Model systems are also examined, and new theoretical techniques are developed. Studies include bulk materials, high-$T_c$ superconductors, fullerides, surface and chemisorbed systems, interfaces, materials under high pressure, clusters, and defects in solids. Close collaboration with experimentalists is maintained comparisons with experiment showing that the calculations are accurate and of predictive power. Bulk materials research is 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. Superconductivity research is focused on mechanisms for high transition temperature and possibilities of superconductivity at high pressures.

132. **CENTER FOR X-RAY OPTICS**
D. Attwood
(510) 486-4463 02-4 $2,021,000

The Center for X-Ray Optics focuses on the development of technologies required for the utilization of emerging sources of soft X-ray and extreme ultraviolet (collectively 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.

**Materials Chemistry - 03**

133. **LOW-TEMPERATURE PROPERTIES OF MATERIALS**
N. E. Phillips
(510) 486-4855 03-1 $155,000

Measurements of low-temperature properties of materials, particularly specific heats but including electrical resistivity and magnetic susceptibility, 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.

134. **CAM ENZYMATIC SYNTHESIS OF MATERIALS PROGRAM**
M. D. Alper, M. Bednarski, J. F. Kirsch, D. E. Koshand, Jr., P. Schultz, C.-H. Wong
(510) 486-6581 03-2 $574,000

Exploitation of recent breakthroughs in bioorganic chemistry, molecular biology, and biochemistry to use 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) 486-0176 03-2 $601,000

Development and synthesis of high performance polymeric materials. Currently the program consists of two projects: anistropic polymeric materials, 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, thermal analysis, and structural theory to elucidate how orientation and stress develop during shaping. The way in which the multi-phasic nature of the polymer melt 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 and adhesion. Polymer synthesis and the development of computational methods for predicting structure development and the onset of dynamical instabilities are integral components of both project areas.

136. **INTERFACIAL MATERIALS AND PROCESSES**
J. D. Porter
(510) 486-7236 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.

137. **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 of surfaces and the mechanical properties of adhesion and friction 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. 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.

138. **ELECTROCHEMICAL PROCESSES**
C. W. Tobias
(510) 486-3764 03-2 $5,000

Novel approaches are explored, and the relevant theoretical framework is established for the control of composition and phase structure in the electrodeposition of alloys. Project is phasing out.

139. **SEMICONDUCTOR THIN FILMS USING NANOCRYSTAL PRECURSORS**
P. Alivisatos
(510) 486-7371 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 denser 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 temperature precursors to thin films.

140. **HIGH-TEMPERATURE THERMODYNAMICS**
L. Brewer
(510) 486-5946 03-3 $35,000

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 equilibration with carbides, nitrides, and oxides are being used to characterize the thermodynamics of these systems.

141. **GROWTH MECHANISMS AT HETEROINTERFACES**
D. Loretto, C. A. Lucas
(510) 486-5960 03-3 $490,000

This initiative is concerned with thin film heterostructures in which there is a large change in electronic structure across the interface. The primary goals are to understand and control growth mechanisms at heterointerfaces and to determine the relationship between the growth mechanism and the atomic and electronic properties of heterointerfaces. Synchrotron X-ray scattering, transmission electron microscopy and X-ray photoelectron spectroscopy are being applied to ionic materials grown on covalent substrates by molecular beam epitaxy. Particular emphasis is placed on combining information from in situ and ex-situ experiments. Experiments are being developed which use ionic-on-covalent thin films to address fundamental scientific problems, including melting phenomena and the role of impurities in epitaxial growth. The high brightness and small beam size of the ALS will be particularly beneficial to the experiments performed in this initiative.

142. **CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES**
D. R. Olander
(510) 486-7055 03-3 $100,000

The overall objective of this program is to characterize the chemical and physical behavior of materials in the high temperature, radiation environment of fission and fusion reactors. The materials of the uranium-based fuels 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 $944,600

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 an undertaking involves the development of new theoretical approaches and experimental methods. Some developments currently underway in this direction are iterative and multiple-pulse sequences, geometric quantum phase, multiple-quantum NMR, zero-field and SQUID-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. The developments above are being used, for example, to study clusters and nanostructures, conductor oxides, silicates, zeolites, aluminophsphates, catalysts, liquid crystals, polymers, icosahedral materials and glasses.

144. **CAM SURFACE SCIENCE AND CATALYSIS PROGRAM**
G. A. Somorjai, A. T. Bell, H. Heinemann, M. B. Salmeron, Y. R. Shen
(510) 486-4053 03-3 $1,044,000

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. Surface instrumentation development is an important part of the project. The Surface Science effort includes studies of atomic scale surface structure of solids and adsorbed 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. The scanning tunneling microscopy (STM) and related techniques (AFM, SFA), digital low energy electron diffraction (LEED) and nonlinear laser optics (SFG and SHG) are the focus of surface instrumentation development.

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 and phosphides, 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 halogen 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**

B. Kincaid - (510) 486-4810
Fax: (510) 486-4960

147. **1-2 GEV SYNCHROTRON LIGHT SOURCE R&D**
B. M. Kincaid
(510) 486-4810 04-1 $22,496,000

The Advanced Light Source project was completed on time and within budget in April of 1993. Key project milestones were met, including the completion of the ALS Storage Ring, and the successful accumulation of stored beam to 65 mA, in excess of the project completion requirement of 50 mA. Within a month, the system design goal of 400 mA stored beam had been reached and exceeded. A great deal of progress in commissioning the accelerator complex was made in the month of April. Five beamlines, including the first two ALS undulator beamlines, are now being installed, with user operations commencing near the end of the summer. A formal close-out project review was held, followed by a project safety review, Key Decision 4 (KD4), formal permission to operate the ALS facility, was granted by the Secretary of Energy in July. Some changes and additions to the facility management have been made, including the positions of Head of Operations, and Head of the Scientific Program. The user research program, based on strict quality assurance and environment, health, and safety protection, has started, with the first outside users arriving in July and August.

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**Metallurgy and Ceramics - 01**

148. **SYSTEMATICS OF PHASE TRANSFORMATIONS IN METALLIC ALLOYS**
L. Tanner
(510) 423-2653 01-1 $524,000

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. Foiles, A. Gonis, E. Sowa, W. G. Wolfer
(510) 423-6547 01-2 $492,000

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 $441,000

The electronic and geometric structures of surfaces, interfaces and ultrathin films constructed from nanocrystalline 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
(510) 423-0570 02-2 $294,000

Linear and nonlinear optical properties of optical materials are investigated including behavior at high laser intensities and during ultrashort pulses of light. 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 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**

152. **NEUTRON IRRADIATION INDUCED METASTABLE STRUCTURES**
K. E. Sickafus, M. Nastasi
(505) 665-3457 01-4 $694,000

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. **STRUCTURAL CERAMICS: INTERFACIAL EFFECTS AND VERY HIGH TEMPERATURE MECHANICAL BEHAVIOR**
T. E. Mitchell, W. R. Blumenthal, A. L. Graham, J. J. Petrovic, D. S. Phillips, A. F. Voter
(505) 667-0938 01-5 $855,000

Our goal is to investigate the mechanical behavior of advanced structural ceramic materials. This presently involves two research programs. The first is associated with deformation and fracture studies of single crystals of oxide and non-oxide ceramics at very high temperatures. The second involves fundamental investigations of the nature and properties of interfaces important to structural ceramic composite systems. Modeling effort are associated with both programs. Materials currently being studied include YAG,$Si_3N_4$, SiC, and $MoSi_2$. Our emphasis is on the mechanical behavior of structural ceramics, including composites, at very high temperatures. The fundamental nature of interfaces and their role in determining mechanical behavior is an important aspect of the research. Investigations being pursued on the deformation behavior of single crystals of $Si_3N_4$, $MoSi_2$, and YAG will be extended to perovskites such as $LaAlO_3$, spinels such as $Mg_2CRO_2$, and other complex oxides and silicides. We will establish melting fabrication facilities for the growth of such crystals and also for eutectic systems. Modeling aspects will emphasize fracture and plasticity effects and atomistic simulations of defects such as dislocations in the very high temperature ceramics, with interatomic potentials developed for these materials which will allow atomistic calculations of features such as dislocation core structures.

154. **METASTABLE PHASES AND MICROSTRUCTURES**
R. B. Schwarz, T. E. Mitchell
(505) 667-8454 01-5 $231,000

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.

155. **MECHANICAL PROPERTIES**
M. G. Stout, U. F. Kocks
(505) 667-4665 01-5 $497,000

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. Phenomenology 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**

156. **CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY**
R. Pynn
(505) 667-6069 02-1 $2,003,000

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 organometallics, atomic arrangements of high-temperature superconductors, actinides and metal hydrides, crystallography at high pressures, texture and preferred orientation in metallurgical and geological samples, the structure of magnetic multilayers, 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.

157. **INTEGRATED MODELING OF NOVEL MATERIALS**
K. S. Bedell, A. R. Bishop, A. F. Voter
(505) 667-6491 02-3 $390,000

This is a core program in condensed matter and materials theory aimed at extending the theory base available for modelling novel electronic 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.

158. **CORRELATED ELECTRONS IN METALS**
Z. Fisk, J. L. Smith, J. D. Thompson
(505) 665-0892 02-2 $251,000

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.

159. **ULTRA-HIGH PRESSURE STUDIES**
D. Schiferl, M. S. Shaw
(505) 665-3150 02-2 $234,000

Studies of phase transformations, crystal structures, changes in bonding, and thermodynamics of simple molecular systems at high pressures (up to 1 Mbar) and extreme temperatures (10-1800 K). Develop theories of phase transformations, structural behavior, and chemical 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.

160. **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 $487,000

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.

161. **HIGH TEMPERATURE SUPERCONDUCTIVITY**
Z. Fisk, A. Arko, P. C. Hammel, I. Raistrick, J. D. Thompson
(505) 665-0892 02-5 $656,000

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.

162. **THERMAL PHYSICS**
G. W. Swift, R. E. Ecke
(505) 665-0640 02-5 $293,000

Experimental investigations of pattern formation and nonlinear dynamics in fluid systems: thermal convection involving nonlinear traveling waves, spatial and dynamic scaling, pattern dynamics; liquid-solid dissolution, mass transfer, turbulence and solid morphology. Experimental and theoretical studies of novel engines: acoustic engines (both heat pumps and prime movers) using liquids and gases; acoustic turbulence; sterling engines using liquids and superfluids: regenerators, heat exchangers, mechanicals, seals.

**Materials Chemistry - 03**

163. **LOW-DIMENSIONAL MIXED-VALENCE SOLIDS**
B. I. Swanson, A. R. Bishop
(505) 667-5814 03-2 $349,000

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**

R. Pynn - (505) 665-1488
Fax: (505) 665-2676

164. **LANSCE OPERATIONS SUPPORT, SPECTROMETER DEVELOPMENT, AND USER SUPPORT**
R. Pynn
(505) 667-6069 04-1 $5,765,000

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. The spectrometers 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 responsibility 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: (303) 231-1997

**Metallurgy and Ceramics - 01**

S. K. Deb - (303) 384-6405
Fax: (303) 231-1271

165. **GROWTH AND PROPERTIES OF NOVEL ORDERED II-VI AND III-V SEMICONDUCTOR ALLOYS**
A. Mascarenhas, J. Olson, A. Zunger
(303) 231-1368 01-1 $588,000

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 II-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, as well as optical consequences of ordering.

**Solid State Physics - 02**

166. **SEMICONDUCTOR THEORY**
A. Zunger
(303) 231-1172 02-3 $221,000

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 quantities (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 INSTITUTE FOR SCIENCE AND EDUCATION

**Oak Ridge, TN 37831**

R. Wiesehuegel - (615) 576-3383

**Metallurgy and Ceramics - 01**

167. **SHARED RESEARCH EQUIPMENT PROGRAM**
N. D. Evans, E. A. Kenik
(615) 576-4427 01-1 $125,000

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, industries, 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 4.0 MeV) Van de Graaff accelerators for Rutherford backscattering and nuclear reaction techniques. A mechanical properties microprobed (Nanoindenter), having high lateral (0.3 m) and depth (0.16 nm) resolution, can characterize elastic/plastic behavior in thin films, layers, interfaces, and other sub-micron features.

## OAK RIDGE NATIONAL LABORATORY

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**Metallurgy and Ceramics - 01**

L. L. Horton - (615) 574-5081
Fax: (615) 574-7659

168. **MICROSCOPY AND MICROANALYSIS**
J. Bentley, E. A. Kenik, M. K. Miller, W. C. Oliver
(615) 574-5067 01-1 $1,139,000

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.

169. **THEORETICAL STUDIES OF METALS AND ALLOYS**
W. H. Butler, C. L. Fu, G. S. Painter, G. M. Stocks
(615) 574-4845 01-1 $840,000

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/LKKR) 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 quantities to understand their mechanical properties. Use of density functional theory and LCAO method to calculate the properties of clusters of atoms. Application of cluster calculations to materials problems such as impurity effects, grain boundary cohesion and grain boundary segregation.

170. **RADIATION EFFECTS**
L. K. Mansur, K. Farrell, E. H. Lee, M. B. Lewis, R. E. Stroller
(615) 574-4797 01-4 $1,589,000

Theoretical and experimental research on defects and microstructures produced by neutron 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 and surface mechanical and physical properties of metallic, and polymeric and ceramic materials; new materials by ion beam processing. Neutron damage in metals and alloys irradiated in HFIR, HFBR and other reactors. Effect of alloying additions; effect of type of irradiation and damage rate; radiation-induced embrittlement, creep and swelling; phase stability under irradiation; relationships 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.

171. **MICROSTRUCTURAL DESIGN OF STRUCTURAL CERAMICS**
P. F. Becher, K. B. Alexander, A. Bleier, C.-H. Hsueh
(615) 574-5157 01-5 $1,011,000

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 to control densification and resultant microstructure and composition in such toughened systems. These micro- and (macro-) scopic characteristics are directly related to phenomena that are controlled during powder synthesis, powder processing, and 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 to provide the fundamental basis for the design and fabrication of advanced ceramics and ceramic composites for elevated temperatures.

172. **FUNDAMENTALS OF WELDING AND JOINING**
S. A. David, J. M. Vitek, T. Zacharia
(615) 574-4804 01-5 $537,000

Correlation between solidification parameters and weld microstructure, distribution, and stability of microphases, microstructure of laser-produced welds, single crystal 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.

173. **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 $1,296,000

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
Fax: (615) 574-4143

174. **STRUCTURES OF ANISOTROPIC COLLOIDAL MATERIALS**
J. B. Hayter, W. A. Hamilton
(615) 576-9300 02-1 $488,000

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.

175. **INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS**
H. A. Mook, J. W. Cable, H. R. Child, J. Fernandez-Baca, R. M. Nicklow, H. G. Smith
(615) 574-5234 02-1 $956,000

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, and magnetic excitations in high-temperature, 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.

176. **STRUCTURE AND DYNAMICS OF ENERGY-RELATED MATERIALS**
H. A. Mook, H. R. Child, R. M. Nicklow, S. Spooner, G. D. Wignall, M. Yethiraj
(615) 574-5234 02-1 $1,340,000

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. Residual stress determinations of ceramic and metal components.

177. **PROPERTIES OF ADVANCED CERAMICS**
J. B. Bates, N. J. Dudney, G. R. Gruzalski, D. C. Lubben, F. A. Modine
(615) 574-6280 02-2 $556,000

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 and electron 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.

178. **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 $488,000

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.

179. **SYNTHESIS AND PROPERTIES OF NOVEL MATERIALS**
L. A. Boatner, M. M. Abraham, J. B. Brewster, B. C. Chakoumakos, Y. Chen
(615) 574-5492 02-2 $1,365,000

Synthesis and characterization of advanced materials including single crystal growth 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 structural characterization 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, actinide-doped single crystals, stainless steels, rapid solidification and solidification microstructures.

180. **PHYSICAL PROPERTIES OF SUPERCONDUCTORS**
D. K. Christen, R. Feenstra, H. R. Kerchner,
C. E. Klabunde, J. R. Thompson
(615) 574-6269 02-2 $439,000

Physical properties of superconductors, particularly high-$T_c$ materials, in various thin-film, single-crystal, melt proposed, 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, 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.

181. **THIN FILMS, SEMICONDUCTOR PHYSICS, AND PHOTOVOLTAIC MATERIALS**
D. H. Lowndes, D. J. Eres, D. B. Geohegan,
G. E. Jellison, D. P. Norton
(615) 574-6306 02-2 $908,000

Time-resolved ellipsometric measurements, time-resolved measurements of pulsed-laser-generated plasmas, pulsed supersonic molecular beam deposition, modulated layered structures, superlattices, fabrication of superconducting and semiconducting thin films by pulsed laser ablation, laser-induced recrystallization of amorphous layers, pulsed-laser bonding of metals to ceramics, thermal and laser annealing of lattice damage in semiconductors, fabrication of solar cells by laser, thick-film and thin-film techniques, effects of point defects and impurities on electrical and optical properties of elemental and compound semiconductors, electrical, optical (including infrared and luminescence spectroscopy), scanning tunneling microscopy, transmission electron microscopy, X-ray scattering, secondary ion mass spectrometry, and Rutherford ion backscattering measurements, dopant concentration profiles, deep-level transient spectroscopy, and absolute quantum efficiency measurements.

182. **ATOMISTIC MECHANISMS IN INTERFACE SCIENCE-DIRECT IMAGING AND THEORETICAL MODELING**
S. J. Pennycook, M. F. Chisholm, D. E. Jesson,
T. Kaplan, V. Y. Millman, M. E. Mostoller,
J. F. Wendelken
(615) 574-5504 02-2 $244,000

Direct imaging of atomic structure and chemistry of interfaces by high-resolution Z-contrast scanning transmission electron microscopy, static and dynamic ab-initio pseudopotential calculations of interface structures and atomistic mechanisms of epitaxial growth, molecular beam epitaxial growth of semiconductors, evolution of surface morphology, strain relaxation, dislocation nucleation, role of surfactants on growth, kinetic ordering, grain boundaries in ceramics and high-temperature superconductors, atomic resolution chemical analysis by electron energy loss spectroscopy, segregation to dislocations, hole concentration mapping in high-temperature superconductors, correlation of microstructure to transport properties, and metal/ceramic interfaces.

183. **X-RAY RESEARCH USING SYNCHROTRON RADIATION**
C. J. Sparks, Jr., G. E. Ice, E. D. Specht
(615) 574-6996 02-2 $444,000

Research focuses on the use of synchrotron radiation as a probe for the study of metal alloys, ceramics, and interfaces, emphasizing the ability to select a particular X-ray energy from the synchrotron radiation spectrum to highlight atomic arrangements of 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. The task includes operation of an X-ray beamline on the National Synchrotron Light Source at Brookhaven National Laboratory. Staff are also involved in the design and construction of an X-ray beamline on the Advanced Photon Source. Important materials' problems under study include: (1) effects of short-range order among atoms on mechanical, chemical and magnetic behavior and on radiation swelling; (2) effects of atomic displacements, caused by bonding and size difference, on energetics of phase stability and materials properties; (3) studies of site substitution on alloying and other defects associated with nonstoichiometry in long-range ordered alloys which affect ductility, ordering temperature and phase stability, and (4) role of atomic-scale structure and chemistry of interfaces in controlling heteropitaxy.

**184. BULK SHIELDING REACTOR SHUTDOWN**
R. L. Stover, R. D. Childs
(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 requires removal of the fuel and other hazardous materials prior to transfer to the Environmental Restoration Program (ERP). Until transfer occurs, surveillance is required in order to meet ES&H requirements and keep the facility and systems structurally sound.

**185. SMALL-ANGLE X-RAY SCATTERING**
G. D. Wignall, J. S. Lin, S. Spooner
(615) 574-5237 02-2 $185,000

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.

**186. THEORY OF CONDENSED MATTER**
J. F. Cooke, H. L. Davis, T. Kaplan, S. H. Liu, G. D. Mahan, M. E. Mostoller, M. T. Robinson, R. F. Wood
(615) 574-5787 02-3 $1,006,000

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 implantation 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, 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.

**187. STRUCTURAL PROPERTIES OF MATERIALS - X-RAY DIFFRACTION**
B. C. Larson, J. D. Budai, J. Z. Tischler
(615) 574-5506 02-4 $390,000

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, 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, 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.

**188. ELECTRON MICROSCOPY OF MATERIALS**
S. J. Pennycook, M. F. Chisholm, D. E. Jesson
(615) 574-5504 02-4 $723,000

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-phase recrystallization; segregation phenomena; electron energy loss spectroscopy; theory of elastic, inelastic, and diffuse scattering of electrons from crystals and defects; Z-contrast image simulation.

**189. INVESTIGATIONS OF SUPERCONDUCTORS WITH HIGH CRITICAL TEMPERATURES**
D. K. Christen, J. Brynestad, D. Budai, B. C. Chakoumakos, H. R. Kerchner
(615) 574-6269 02-5 $585,000

Studies of superconducting materials with high transition temperatures. Synthesis, characterization, and analysis 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.

190. **SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND RESEARCH CENTER**
D. B. Poker, T. P. Sjoreen, J. M. Williams, S. P. Withrow
(615) 576-8827 02-5 $1,620,000

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.

191. **ION BEAM ANALYSIS AND ION IMPLANTATION**
C. W. White, T. E. Haynes, O. W. Holland, R. A. Zuhr
(615) 574-6295 02-5 $897,000

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, to the formation of nonlinear optical materials 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 ions (10-200 eV) to alter surface atom mobilities and phase formation.

192. **SURFACE PHYSICS AND CATALYSIS**
D. M. Zehner, A. F. Baddorf, H. L. Davis, J. F. Wendelken
(615) 574-6291 02-5 $878,000

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, scanning tunneling microscopy (STM), and computer simulations for surface crystallography studies with emphasis on surfaces which either reconstruct or have interplanar spacings different from those of the bulk, LEED, Auger Electron Spectroscopy (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.

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**Materials Chemistry - 03**

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193. **CHEMISTRY OF ADVANCED INORGANIC MATERIALS**
C. E. Bamberger, J. Brynestad, L. Maya, C. E. Vallet
(615) 574-4944 03-1 $1,056,000

Systematic studies of electrocatalysts for various reactions of interest in energy conversion/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 electrocatalytic processes (reaction kinetics and mechanism, electrocatalytic activity, electronic and structural properties) by electrochemical techniques, photoacoustic/photothermal-deflection spectroscopies, and STM. Synthesis of whiskers and platelets for direct use as reinforcing agents in composite materials or as precursors in pseudomorphic conversions, i.e., reactions in which the product retains the morphology of the precursor; Emphasis is on conversions of oxides to carbides and nitrides in gas-solid and molten salt reactions. 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 in the metal-C-N-B regime. 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; aerosol synthesis of complex powders.

194. **STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS**
B. K. Annis, A. Habenschuss, D. W. Noid, B. G. Sumpter, B. Wunderlich
(615) 574-6018 03-2 $1,123,000

Characterization of polymers and composites at the molecular level by small-angle and wide-angle neutron and X-ray scattering, thermal and mechanical analysis, atomic force microscopy, NMR spectroscopy, 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.

195. **NUCLEATION, GROWTH, AND TRANSPORT PHENOMENA IN HOMOGENEOUS PRECIPITATION**
M. T. Harris, O. A. Basaran, C. H. Byers
(615) 574-1275 03-2 $289,000

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. The focus of the program entails investigation of metal alkoxide/metal salt reactions and reactants-solvent interactions (i.e., short-range bonding) which affect the characteristics of the particles formed. Another important aspect of this effort is the 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) are important features of this research.

196. **THERMODYNAMICS AND KINETICS OF ENERGY-RELATED MATERIALS**
T. B. Lindemer
(615) 574-6850 03-2 $303,000

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 (Y, lanthanide) barium-copper-oxygen systems. These efforts are providing a heretofore unavailable description of these oxides.

197. **BLENDS OF MACROMOLECULES WITH NANOPHASE SEPARATION**
G. D. Wignall, J. G. Curro (SNL/A), K. S. Schweizer (Univ. of ILL/MRL)
(615) 574-5237 03-2 $487,000

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.

**Facility Operations - 04**

198. **ADVANCED NEUTRON SOURCE**
C. D. West, M. L. Gildner, J. B. Hayter, B. H. Montgomery, D. L. Mosses, D. L. Selby, P. B. Thompson
(615) 574-0370 04-1 $20,559,000

Preconstruction R&D associated with the Advanced Neutron Source (ANS) at ORNL. Core physics, neutronics, and thermal hydraulics for a conceptual core design. Operation of corrosion and thermal-hydraulic test loop to study oxide formation and growth. Construction of a loop to measure the effects of channel blockage on core cooling.

Construction of a stand for testing control rod release hatch mechanisms. $U_3Si_2$ 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. Preparation of a draft Environmental Impact Statement.

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### Metallurgy and Ceramics - 01

199. **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 $391,000

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 allows evaluation of packing efficiency and correlation to chemical functionality of tailored inorganic polymer dispersants. Behavior of bound polymer in the greenbody to temperature during sintering is a principal area of active research. 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.

200. **FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS**
R. H. Jones, C. H. Henager Jr., E. P. Simonen, C. F. Windisch, Jr.
(509) 376-4276  01-2 $419,000

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. 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 transient electrochemical analysis.

201. **CHEMISTRY AND PHYSICS OF CERAMIC SURFACES**
L. R. Pederson, B. C. Bunker, K. F. Ferris
(509) 375-2731  01-3 $373,000

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 modelling activities emphasize ab initio electronic structure and molecular dynamics approaches, and include the development of methodologies for large-scale assemblies.

202. **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 modelling. Research includes examination of radiation effects on grain boundary chemistry, matrix and interfacial deformation processes, crack-tip phenomena, and material electrochemical behavior. 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 models are being evolved so that radiation effects on local material microstructure, microchemistry, deformation and electrochemistry can be assessed in relation to crack propagation mechanisms.

203. **IRRADIATION EFFECTS IN CERAMICS**
W. J. Weber, N. J. Hess
(509) 375-2299 01-4 $262,000

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, stability, and 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**

204. **THIN FILM OPTICAL MATERIALS**
G. J. Exarhos, K. F. Ferris, N. J. Hess
(509) 375-2440 02-2 $231,400

Theoretical and experimental investigations of basic materials properties which control the linear and nonlinear optical behavior and phase stability 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, electron microscopy, and atomic force microscopy, are integrated into these models. Ellipsometry and optical transmission/reflection measurements on supported films are used to determine complex refractive indices; the nonlinear response is investigated by means of harmonic mixing methods. Materials studied include oxides, nitrides, garnets, and inorganic polymers.

**Materials Chemistry - 03**

205. **CERAMIC COMPOSITE SYNTHESIS UTILIZING BIOLOGICAL PROCESSES**
P. C. Rieke, B. C. Bunker, A. A. Campbell, A. I. Caplan, G. E. Fryxell, G. L. Graff, A. H. Heuer (Case Western Res. Univ.)
(509) 375-2833 03-1 $527,000

Processing routes have been developed to make ceramic thin films or composites via controlled nucleation and growth from aqueous solutions onto functionalized interfaces. The techniques, called biomimetic processing, stimulate nucleation and growth on substrates by using functional groups that mimic the behavior of biomineralization proteins. This program has demonstrated that high-quality ceramic films can be grown on plastics and other materials at temperatures below 100°C. Conformal coatings with unique oriented and/or nanocrystalline microstructures can be produced. The current emphasis of the program is to establish mechanisms for the surface nucleation and growth processes controlling biomimetic depositions using studies on self-assembling monolayers, Langmuir-Blodgett films, and colloidal particles as substrates.

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**Metallurgy and Ceramics - 01**

206. **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 $523,000

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.

207. **PHYSICS AND CHEMISTRY OF CERAMICS**
D. W. Schaefer, R. A. Assink, C. J. Brinker, R. K. Brow, P. F. Green, A. J. Hurd, R. W. Schwartz, J. A. Voigt
(505) 844-7937 01-2 $0

Due to their refractory nature, processing from solution has been intrinsic to ceramics since the prehistoric times. This program seeks to characterize and model the chemical and physical processes that link solution precursors to final properties. Systems of interest include controlled pore solids, films, fibers and polycrystalline ceramics useful as superconductors, catalysts and ferroelectrics. Structure on multiple length scales is essential to ceramic processing. For complex materials control of structure from 10 A to 10 mm is critical to performance. We use a battery of tools including NMR, small-angle neutron scattering, chemical imaging and imaging ellipsometry to establish structure of solutions, films, and monoliths. We seek to measure and model the effects of processing on pore formation, crystallite growth and sintering. Since most of our systems are amorphous at some stage, we are exploring the nature of glassy materials. We are particularly interested in the effect of network topology on relaxation processes, including the glass transition itself. We are developing a set of new tools including dynamic mechanical analysis, Brillouin scattering and high-resolution inelastic neutron scattering.

208. **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, C. H. Seager, H. J. Stein, W. R. Wampler
(505) 844-6076 01-3 $882,000

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. Ion beams are used in conjunction with such techniques as TEM, X-ray scattering, IR spectroscopy, AES, capacitance-voltage analysis, DLTS, and mechanical testing to explore the properties of beam-synthesized materials and to illuminate a wide range of fundamental atomic processes in solids.

Representative areas of research include ion-beam synthesis of nanostructures with novel chemical and electrical properties in semiconductors, ECR-plasma growth of superior new dielectrics, the formation by ion implantation and pulsed-laser deposition of new AL alloys with very high strengths, and fundamental studies of the interactions of H with semiconductors.

209. **ADVANCED GROWTH TECHNIQUES FOR IMPROVED SEMICONDUCTOR STRUCTURES**
S. T. Picraux, D. K. Brice, S. A. Chalmers, E. Chason, B. W. Dodson, J. A. Floro, B. Swartzentruber, J. Y. Tsao
(505) 844-7681 01-3 $389,000

Advanced growth techniques are studied for the synthesis of new and improved epitaxial semiconductor heterostructures. 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 correlation with growth parameters. Theoretical studies model the growth processes and address growth mechanisms in order to interpret and guide the experimental studies.

210. **STRAINED-LAYER SEMICONDUCTOR MATERIALS SCIENCE**
P. L. Gourley, I. J. Fritz, E. D. Jones, S. K. Lyo, J. S. Nelson, R. Schneider, Jr., M. B. Sinclair
(505) 844-5806 01-5 $375,000

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 coordinates semiconductor physics and materials science to produce new semiconductor materials with useful electronic properties not available in bulk compound semiconductor crystals. This program investigates fundamental material properties including band structure, electronic transport, crystal stability, optical transitions, and nonlinear optical properties. Both theoretical and experimental understanding are emphasized. The materials under study have a wide range of applications for high speed switching and microwave technologies, optical detectors, lasers, and optical modulation and switching.

**Solid State Physics - 02**

211. **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 $632,000

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.

212. **PHYSICS AND CHEMISTRY OF NOVEL SUPERCONDUCTORS**
E. L. Venturini, B. W. Dodson, B. Morosin, P. P. Newcomer, D. L. Overmyer, J. E. Schirber, M. P. Siegal, E. B. Stechel
(505) 844-7055 02-2 $612,000

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.

213. **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 $503,000

This program investigates boron-rich solids which are refractory materials with unconventional 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**

214. **CHEMICAL VAPOR DEPOSITION SCIENCES**
P. E. Sherick, 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 $792,000

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 that 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.

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### Metallurgy and Ceramics - 01

W. Wolfer - (510) 294-2307
Fax: (510) 294-3231

215. **SURFACE, INTERFACE, AND BULK PROPERTIES OF ADVANCED CERAMICS**
R. H. Stulen, K. F. McCarty
(510) 294-2070    01-1 $182,000

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. Emphasis is placed on two important material systems: (1) ultrahard ceramics and (2) high-temperature superconductors. We are utilizing the emerging technique of pulsed laser deposition (PLD) for film synthesis. Currently, we strive to develop a fundamental understanding of what processes control the formation of a metastable phase, such as (diamond-like) cubic boron nitride (cBN), over formation of the stable (graphite-like) phase. By determining and controlling the film nucleation mechanism, and controlling the species and energy distribution of the ions, we strive to produce phase-pure films of cBN using ion-assisted PLD. Using in situ diagnostics in the growth chamber, we will determine the relationship between the deposition parameters and the film properties. We explore the relationship between phonon structure, electronic structure, physical structure, and the transition temperature of high-$T_c$ superconductors using Raman spectroscopy. Raman-active phonons are identified through polarization analysis of single crystals. Temperature-dependent measurements of light scattering from the conduction electrons and the phonons allow the energy gap to be determined, along with its anisotropy. We determine how doping affects the electron-phonon coupling, the electronic Raman scattering, and the temperature dependence of the phonon linewidths.

216. **DEFECTS AND IMPURITIES IN SOLIDS/COMPUTATIONAL MATERIALS SCIENCE/VISITING SCIENTIST PROGRAM**
W. G. Wolfer, S. Bailes, D. C. Chrzan, M. S. Daw, S. M. Foiles, J. C. Hamilton, R. Q. Hwang, M. J. Mills, A. A. Quong
(510) 294-2307    01-2 $1,224,000

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 density matrix (DM) 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 investigated 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 and to industrial research and development laboratories is conducted through the Visiting Scientist Program.

217. **ALLOY THEORY**
D. D. Johnson, J. D. Althoff, F. J. Pinski (Univ. of Cinn.)
(510) 294-2751    01-3 $488,000

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**

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Fax: (510) 294-3231

218. **ADVANCED OPTICAL DIAGNOSTICS FOR INTERFACES AND THIN FILMS**
R. H. Stulen, R. J. Anderson
(510) 294-2070 02-2 $235,000

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) photoluminescence spectroscopy to probe electronic structure and defects of bulk materials and thin films, 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: (415) 926-4100

**Facility Operations - 04**

219. **RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES**
A. I. Bienenstock, H. Winick
(415) 926-3153 04-1 $2,540,000

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 superconductors and 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. Photoelectron spectroscopic studies of catalysts. Development and improvement of accelerators and insertion devices for synchrotron radiation production. Development of Laue 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.

## UNIVERSITY OF ALABAMA
**1150 10th Avenue South**
**Birmingham, AL 35294**

220. **MIGRATION OF CONSTITUTIONALLY LIQUIDATE FILMS**
R. G. Thompson, Department of Materials Science and Engineering
(205) 934-8450

B. Radhakrishnan, Department of Materials Science and Engineering
(205) 934-8450 01-5 $66,000

Study of the migration of precipitate boundaries accompanying constitutional liquid film migration (CLFM). Demonstrate the occurrence of CLFM in binary alloys. Extend the studies to ternary systems containing the binaries. Thermal simulation will use a Gleeble device. Characterization techniques include quantitative microscopy to determine grain size, number of grains per unit volume, area fraction of migrated area, average migration distance, and volume fractions of precipitate and liquid and TEM to determine concentration gradients.

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

221. **STRUCTURE, STOICHIOMETRY AND STABILITY IN MAGNETOPLUMBITE AND β-ALUMINA TYPE CERAMICS**
A. N. Cormack, Department of Ceramic Science and Engineering
(607) 871-2180 01-1 $51,001

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**

222. **SOLID ELECTROLYTES AND IMPACT-RESISTANT CERAMICS**
C. A. Angell, Department of Chemistry
(602) 965-7217 01-1 $149,848

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.

223. **HIGH RESOLUTION ENERGY LOSS RESEARCH: SI COMPOUND CERAMICS AND COMPOSITES**
R. W. Carpenter, Center for Solid State Science
(602) 965-4549

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

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.

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

Studies of surface structures of oxides and metals and of solid-solid interfaces using a range of advanced electro-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**

225. **EARLY STAGES OF NUCLEATION**
M.C. Weinberg, Department of Materials Science and Engineering
(602) 621-6909 01-1 $124,366 (14 months)

Nucleation of glass-in-glass phase separation. Electron microscopy, Raman spectroscopy, and small angle X-ray scattering techniques will be used to study the nucleation rates and compare them with the predictions of Classical Nucleation Theory.

226. **ARTIFICIALLY STRUCTURED MAGNETIC MATERIALS**
C. M. Falco, Department of Physics
(602) 621-6771

B. N. Engel, Department of Physics,
(602) 621-2171 02-2 $90,000

Emphasis on the measurement of magnetic properties of well-characterized, artificially structured, metallic monolayers, multilayers and superlattices, with a major thrust being a study of those systems where experimental data will contribute to an understanding of interface magnetic anisotropy. Fabrication of experimental samples by molecular beam epitaxy (MBE) and multi-target sputtering. Sample characterization by use of X-ray diffraction, reflected high-energy and low-energy electron diffraction (RHEED and LEED), scanning tunneling and atomic force microscopy (STM and AFM), Rutherford backscattering (RBS), scanning and transmission electron microscopy (SEM and TEM), and X-ray photoelectron spectroscopy (XPS). Determination of magnetic properties by surface magneto-optic Kerr effect (SMOKE), variable-temperature vibrating sample magnetometry (VSM), Brillouin light scattering, neutron scattering, and synchrotron photoemission studies. Efforts in developing artificially structured magnetic materials with improved properties.

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

227. **X-RAY SPECTROSCOPIC INVESTIGATION OF AMORPHIZED MATERIALS**
R. B. Greegor, Department of Physics
(206) 773-5737 01-1 $46,530 (10 months)

XANES/EXAFS data analysis proton-irradiated intermetallics, uranium borosilicate glasses reacted in water, site speciation in waste forms (synroc, in situ vitrified glass) and zircons (crystalline, metamict and temperature annealed) will be performed. Work on zircons will be extended to include scattering measurements (RDF, DAS, DDF) to better characterize the distorted, anharmonic pair-distribution function in amorphized samples of this system. Radiation damage from the oxygen (and possible Si) site in metamict zircons will be accomplished using recently developed methods which allow samples that are not ultra high vacuum compatible to be examined using ultra soft (25 - 1300 eV) fluorescent measurements to obtain FYNES and EXAFS spectra.

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

228. **THE HEAVY ELECTRON STATE**
A. Auerbach, Department of Physics
(617) 353-5787 02-3 $30,000

The 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.

229. **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 $117,800

Use of scattered spin-polarized metastable $He(_{23}S)$ atoms from surfaces both elastically and inelastically, to study the structural, dynamic and magnetic trends of the 3D transition metal overlayers-Cu, Au, Ag and Cr on Pd(111) and Pd(110) substrates; and Pd and Cu on Nb(110) substrate. Magnetic properties will be studied in the newly constructed Spin-Polarized

Metastable He (SMPH) facility. Spin-ordering in NiO, MnO, and CoO will be investigated. Large-scale canonical molecular dynamics simulations combining a hybrid Nose-Hoover thermostat and Andersen's constant pressure algorithms will parallel the experiments.

## BRANDEIS UNIVERSITY
**Waltham, MA 02254**

230. **ORDERING IN CRYSTALLINE AND QUASICRYSTALLINE ALLOYS: AN ATOMISTIC APPROACH**
B. Chakraborty, Department of Physics
(617) 736-2835 01-1 $60,000

Theoretical effort based on Effective Medium Theory (EMT). Study of phase stability and kinetics of ordering in crystalline and quasicrystalline alloys. Comparison with the KKR-CPA approach. Applied to Cu-Au alloys and intermetallics exhibiting quasicrystalline order.

## BRINGHAM YOUNG UNIVERSITY
**Provo, UT 84602**

231. **MICROSTRUCTURAL DEPENDENCE OF CAVITATION DAMAGE IN POLYCRYSTALLINE MATERIALS**
B. L. Adams, Department of Manufacturing Engineering and Engineering Technology
(801) 378-6177 01-2 $42,557

A detailed correction between crystallographic aspects of grain boundaries and their propensity to creep cavitate in Cu. Serious attention is given to the requirement of obtaining data more rapidly. Automation may realize a speedup factor of about 60 in obtaining the required data, and this would enable a much greater clarity of the damage heterogeneity. This will enable a more thorough investigation into the mechanisms which contribute to creep damage and which control the time-to-fracture. Additionally, this may eventually lead to a refining of the current theory of void growth to include grain boundary structure, thereby more accurately predicting the useful life of structural components. The data obtained may be useful as an engineering tool aimed at controlling the processing of structural materials to obtain maximum resistance to cavitation damage.

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

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

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

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

## 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. Makherjee, 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. **RADIATION DAMAGE AND DECOMPOSITION OF CERAMICS BY MICROSCOPY**
D. G. Howitt, Department of Mechanical Engineering
(916) 752-1164 01-4 $62,000 (9 months)

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 CRACK GROWTH UNDER MIXED-MODE LOADING CONDITIONS**
J. C. Earthman, Department of Mechanical and Aerospace Engineering
(714) 856-5018

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

Mechanisms of high-temperature crack growth under different multiaxial stress states in 304 SS and TiAl. Examination of cavity density, cavity distribution, cavitating grain boundary facet size and orientation, and rupture surface topography for three states of stress. Evaluation of effect of multiaxial stresses on the role of intergranular particles. Analysis of crack tip stress states using finite element techniques.

236. **OPTICAL SPECTROSCOPY AND SCANNING TUNNELING MICROSCOPY STUDIES OF MOLECULAR ADSORBATES AND ANISOTROPIC ULTRATHIN FILMS**
J. C. Hemminger, Department of Chemistry
(714) 856-6020 02-2 $120,000

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. **THEORETICAL STUDIES OF ELECTRON SCATTERING SPECTROSCOPIES OF MAGNETIC SURFACES AND ULTRA THIN FILMS**
D. L. Mills, Department of Physics
(714) 856-5148 02-3 $104,000

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
(310) 825-7011 01-4 $87,983

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**

240. **SUPERCONDUCTIVITY AND MAGNETISM IN D- AND F-ELECTRON MATERIALS**
M. B. Maple, Department of Physics
(619) 534-3968 02-2 $300,000

Research on superconductivity and magnetism in d- and f-electron materials will be performed. Emphasis will be on two classes of materials, the high critical temperature copper oxide superconductors and heavy electron rare earth and actinide compounds. Measurements will be made on the intrinsic anisotropic superconducting and normal state properties. Single crystals and magnetically-aligned specimens of the electron-doped copper oxide superconductors and Pr-doped 1-2-3 compounds will be investigated. Measurements on single crystals and polycrystals of heavy Fermion superconductors will be made to determine the role, if any, of a multicomponent, anisotropic superconducting order parameter and possible multiple superconducting transitions. Experiments will be performed to characterize the two-channel quadrupolar Kondo effect in the $Y_{1-x}U_xPd_3$ system.

241. **PREPARATION AND CHARACTERIZATION OF SUPERLATTICES**
I. K. Schuller, Department of Physics
(619) 534-2540 02-2 $90,000

Preparation and characterization of superlattices that have atomic constituents which do not usually form solid solutions. Search for new superlattices; studies of relationships between epitaxial and superlattice growth; comparison of samples prepared by sputtering and thermal evaporation. Preparation of some samples by molecular beam epitaxy (MBE). Characterization of superlattice samples by X-ray diffraction, scanning tunneling microscopy, electron microscopy, and in situ, relatively high energy electron diffraction (RHEED). Other properties, such as transport, magnetic, optical, and superconducting, are measured in collaboration with other investigators. Some of the specific superlattices studied are Pb/Ge, Fe/Cr, Ni/NiO, Co/CoO, FeMn/FeNi alloys, and some transition metal/rare earth systems.

242. **ION MIXING OF SEMICONDUCTOR LAYERED-STRUCTURES**
S. S. Lau, Department of Electrical Engineering and Computer Sciences
(619) 534-3097 02-4 $25,000 (3 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 to be 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**

243. **FUNDAMENTAL STUDIES OF THE INTERRELATIONSHIP BETWEEN GRAIN BOUNDARY PROPERTIES AND THE MACROSCOPIC PROPERTIES OF POLYCRYSTALLINE MATERIALS**
D. R. Clarke, Materials Department
(805) 893-4685 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 boundaries in bicrystals as a function of bicrystallography 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.

244. **THEORIES OF PATTERN FORMATION AND NONEQUILIBRIUM PHENOMENA IN MATERIALS**
J. S. Langer, Department of Physics
(805) 893-2280 02-3 $100,000

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.

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

R. J. Sugar, Physics Department
(805) 893-3469 02-3 $90,000

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

246. **MOLECULAR PROPERTIES OF THIN ORGANIC INTERFACIAL FILMS**
J. Israelachvili, Department of Chemical and Nuclear Engineering
(805) 893-8407 03-1 $180,000

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.

247. **INTERFACIAL PROPERTIES OF HYDROSOLUBLE POLYMERS**
P. A. Pincus, Materials Department
(805) 893-4685 03-2 $45,000 (6 months)

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**

248. **STATICS AND DYNAMICS IN SYSTEMS WITH FRUSTRATION AND/OR RANDOMNESS**
D. Belanger, Department of Physics
(408) 459-2871 02-1 $88,000

Neutron scattering, light scattering and pulsed specific heat techniques are applied to magnetic systems with frustrated interactions, random interactions, or both. Systems being investigated include dilute antiferromagnets such as $Fe_xZn_{1-x}F_2$, which exhibits random-exchange behavior in zero applied field and random-field behavior in an applied field, and structural systems such as $Dy(As_xV_{1-x})O_4$. Thin epitaxial films are being examined; magnetic X-ray scattering in thin films is being investigated.

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

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

Study of kinetic 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.

250. **STUDIES OF ALLOY STRUCTURES AND PROPERTIES**
W. L. Johnson, Division of Engineering and Applied Science
(818) 395-4433 01-1 $397,740

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.

251. **IRRADIATION - INDUCED TRANSFORMATIONS IN THIN FILMS**
H. A. Atwater, Department of Applied Physics
(818) 356-2197 01-4 $95,054

Investigations focused on two areas, one an ongoing effort and other quite new. The ongoing effort is directed at quantification of the early stages of nucleation, an area that has largely eluded direct observation since the inception of research into the structure and stability of materials. The aim to probe the evolution of crystal cluster size distribution in silicon at -or very near the critical size for thermodynamic stability. This will determine in what manner nucleation kinetics conform to or depart from the widely-used but little-supported classical theory of nucleation. Principal new effort will be an investigation of radiation-induced precipitation of nanometer-scale clusters of silicon and *germanium from supersaturated solid solutions of Si* and Ge in $SiO_2$. These systems bear strong analogy to irradiation-induced nucleating of crystal Si in amorphous Si, as both involve quantifiable thermodynamic driving forces, and transport of defects in an amorphous matrix. A key difference, however, is that precipitation involves atomic transport of species which are not part of the matrix, unlike the previous work on crystallization of amorphous silicon. In addition, there has recently been considerable excitement over the anomalous photoluminescence exhibited by nanometer-scale crystal of group IV semiconductors. So far the mechanisms for luminescence remain unclear, but a key step in addressing the luminescence mechanism is the control of crystal size. Dramatic results in control of crystal size in Si nucleation suggest the possibility of similar effects during irradiation-induced precipitation.

252. **MELTING IN ADSORBED FILMS**
D. L. Goodstein, Department of Physics and Applied Physics
(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**

253. **PRESSURE-INDUCED AMORPHIZATIONS OF SILICA 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.

254. **THE ROLE OF MICROSTRUCTURAL PHENOMENA IN MAGNETIC MATERIALS**
D. E. Laughlin, Department of Materials Science and 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.

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 $95,106

Combined *experimental and theoretical study of the* relation between composition and structure of solid/solid interphase boundaries. Experimental work to be carried out by three approaches; 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 appropriate dopants. Modelling of interphase boundary structure and composition will be performed by Monte Carlo techniques.

256. **THEORETICAL MODELS FOR THE ULTIMATE STRENGTH AND FLAW RESISTANCE OF UNDIRECTIONALLY-REINFORCED CERAMIC-MATRIX COMPOSITES**
P. S. Steif, Department of Mechanical Engineering
(412) 268-3507 01-2 $0 from prior year

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

## CASE WESTERN RESERVE UNIVERSITY
**10900 Euclid Avenue**
**Cleveland, OH 44106**

257. **DISLOCATIONS AND POLYTYPIC TRANSFORMATIONS IN SIC**
P. Pirouz, Department of Materials Science and Engineering
(216) 368-6486 01-1 $102,427

Experimental and theoretical study of mechanisms for polytypic transformations of a-SiC. Compressive deformation of 6H SiC single crystals at temperatures up to 1700°, inert atmospheres and nitrogen environments; TEM observation of deformation modes and polytype development. Annealing experiments on 6H-SiC single crystals and 3C-SiC films in inert gas and nitrogen environments; effects of dislocations introduced by surface scratches investigated; TEM determination of polytype development. Determination of the presence of residual dislocations on cross-slip planes following polytypic transformation; thick sections examined by HVEM. Theoretical analysis of formation of Frank-Read dislocation loops and cross-slip of dissociated screw dislocations, effects of stress and temperature; quantitative analysis of mechanism of cross-slip; determination of the activation energy for the motion of partial dislocations.

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

258. **HIGH-TEMPERATURE THERMOCHEMISTRY OF TRANSITION METAL BORIDES AND SILICIDES**
O. J. Kleppa, The James Franck Institute
(312) 702-7198 01-3 $82,060

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, borides, aluminides, and germanides.

## UNIVERSITY OF CINCINNATI
**498 Rhodes Hall (ML-12)**
**Cincinnati, OH 45221**

259. **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) 556-5172 01-5 $70,400

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 (LEHMAN COLLEGE)
**Bedford Park Blvd West**
**Bronx, NY 10468**

260. **STATICS AND DYNAMICS OF THE MAGNETIC FLUX IN HIGH TEMPERATURE SUPERCONDUCTORS**
E. M. Chudnovsky, Department of Physics and Astronomy
(718) 960-8770 02-3 $34,877

Theoretical investigation of the static and dynamic behavior of magnetic flux lines in high-temperature superconductors. Static behavior interpreted via a comprehensive theory of a Hexatic Vortex Glass to represent the vortex lattice of the flux lines, and use of numerical simulations to study the vortex lattice with extended orientational order but only limited translational order. Investigation of the dynamics of magnetic relaxation in two-dimensional, layered superconductors and its relationship to recent experimental results. Attention given to the high temperature depinning of vortices due to their annihilation with antivortices, with tests to determine if this effect is responsible for the irreversibility line in high-temperature superconductors. Study of quantum tunneling of vortices through pinning barriers and their diffusion due to quantum unbinding of vortex pairs.

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

261. **NONLINEAR DYNAMICS AND PATTERN SELECTION AT THE CRYSTAL - MELT INTERFACE**
H. Z. Cummins, Department of Physics
(212) 650-6921 02-2 $108,000

Dynamics and pattern formation at the crystal-melt interface during the free solidification of pure materials and the directional solidification of binary alloys. Special attention given to instabilities, growth of small fluctuations, steady-state dendritic growth, dendritic sidebranching by perturbations, and parity breaking tilt bifurcations. Investigations conducted by use of light scattering and videomicroscopy techniques. Thermal perturbations on the crystal growth process introduced by laser pulses.

262. **MAGNETIC PROPERTIES AND CRITICAL BEHAVIOR OF THE CONDUCTIVITY NEAR THE M-I TRANSITION**
M. P. Sarachik, Department of Physics
(212) 650-5618 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 different uniaxial stress and in varying magnetic fields.

263. **TRANSPORT IN SMALL AND/OR RANDOM SYSTEMS**
M. Lax, Department of Physics
(212) 650-6864 02-3 $84,000

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 is reexamined and partial noise in the presence of feedback evaluated.

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

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

To synthesize and study the properties of new rare-earth-transition metal permanent magnet systems; to further elucidate the sputter process growth dynamics which allow specifically textured magnetic films of different systems to be synthesized; and to make layered geometry structures utilizing systems with in-plane and perpendicular-to-the-plane magnetic anisotropies.

265. **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) 520-5125 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**

266. **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 from prior year

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 modelling 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. Modelling 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.

## CLEMSON UNIVERSITY
**Clemson, SC 29634**

267. **CHARACTERIZATION AND THERMOPHYSICAL PROPERTIES OF BI-BASED CERAMIC SUPERCONDUCTORS, PART B**
M.V. Nevitt, Department of Physics and Astronomy
(803) 656-5303 01-3 $139,240

The measurement of the heat capacity of YBCO and BISCCO single crystal superconductors are performed. Because available single crystals are small, microcalorimetry techniques, suitable for measuring submilligrain samples, are used. Thermophysical measurements are expected to provide insight into the origin of the superconductivity state, and characterizing the electron-phonon-interaction.

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

268. **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 from prior year

Composite modelling 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.

269. **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.

## COLORADO STATE UNIVERSITY
**Fort Collins, CO 80523**

270. **PROPERTIES OF MOLECULAR SOLIDS AND FLUIDS AT HIGH PRESSURE AND TEMPERATURE**
R. D. Etters, Department of Physics
(303) 491-5374 02-3 $15,000

Theoretical calculation of the properties of molecular solids and fluids over broad ranges of high temperatures and pressures. Properties of interest are as follows. Solids: equilibrium structures and orientations, lattice vibrational and vibrational mode frequencies, intramolecular vibron frequencies, sound velocities, equations of state, compressibilities, and structural and orientational phase transitions. Fluid phase: equations of state, vibron frequencies, the melting transition, specific heats, compressibilities, second viral coefficients, viscosities and other transport properties, and the nature of orientational and magnetic correlations. Techniques used include multi-dimensional optimization strategies, self-consistent lattice dynamics, constant pressure and constant volume Monte Carlo (i.e., variable metric) computation, mean field and classical perturbation methods. Systems studied include $N_2$, $O_2$, CO, $CO_2$, $F_2$, $N_2O$, $I_2$, $Cl_2$, $Br_2$, HI, HBr, and $H_2$. Attention is given to connections with combustion and detonation phenomena, and to synthesis of new materials. Collaboration with theoretical work and close correlation with experimental programs at LANL and LLNL continues.

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

271. **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 "universal" relaxation effect in simple ionic materials over a wide temperature regime.

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

272. **TRANSFORMATION TOUGHENING**
P. C. Clapp, Department of Metallurgy
(203) 486-4620 01-1 $130,337

Development of theory of transformation toughening that includes contribution of the shear components of the transformation 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 nonlinear 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 nonlinear elastic effects.

273. **SYNCHROTRON RADIATION STUDIES OF LOCAL STRUCTURE AND BONDING IN HIGH $T_c$ SUPERCONDUCTING OXIDES, TRANSITION METAL ALUMINIDES AND SILICIDES**
J. I. Budnick, Department of Physics
(203) 486-5541 02-2 $80,000 from prior year

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**

274. **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.

275. **STUDIES OF THE III-V COMPOUNDS IN THE MEGABAR RANGE**
A. L. Ruoff, Department of Materials Science and Engineering
(607) 255-4161 01-1 $94,720 (10 months)

Crystal structure changes in Group IV elements and III-IV compounds as a function of pressure; transformations from four-fold to six-fold, eight-fold and twelve-fold coordination. Loading and unloading experiments; EDXD and angle-dispersive studies, optical studies, TEM, XAFS and Raman spectroscopy; visible and near infrared reflectivity of high pressure metallic phases of specific III-IV compounds to characterize spacing determined over a broad range of pressure to verify and evaluate theoretical models.

276. **EXPERIMENTAL STUDIES OF THE STRUCTURE, CHEMISTRY, AND PROPERTIES OF GRAIN BOUNDARIES**
S. L. Sass, Department 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.

277. **UHV-STEM STUDIES OF MATERIALS**
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

Extension of the present capabilities of quantitative microscopy with atomic resolution and application to an analytical study of $Ni_3Al$ and NiAl. The studies of the electron scattering processes from perfect crystal studies will be extended to include defects (dislocations and point defects) and grain boundaries. These studies will provide the key to the interpretation of annular dark field imaging, X-ray spectroscopy and EELS experiments.

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

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

279. **SURFACE PHASES, SURFACE DEFECTS AND INITIAL STAGES OF OXIDATION**
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.

280. **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.

281. **THE GEOMETRY OF DISORDER: THEORETICAL INVESTIGATIONS OF QUASICRYSTALS AND FRUSTRATED MAGNETS**
C. L. Henley, Department of Physics
(607) 255-5056 02-3 $19,035 (6 months)

Investigate quasicrystal geometry to compute phason elastic constants, investigate 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.

282. **SYNTHESIS AND PROPERTIES OF NOVEL METAL CLUSTER AND NETWORK PHASES**
F. J. DiSalvo, Department of Chemistry
(607) 255-7238 03-1 $81,053 (6 months)

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 chacogenide 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**

283. **THE RELATIONSHIP BETWEEN INTERGRANULAR FRACTURE AND GRAIN BOUNDARY STRUCTURE/CHEMISTRY IN B2 INTERMETALLICS**
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, $\text{sigma}_y = \text{sigma}_o + Kd^{-1/2}$, 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.

284. **THE NOTCH SENSITIVITY OF INTERMETALLIC COMPOUNDS**
E. M. Schulson, Thayer School of Engineering
(603) 646-2888 01-2 $173,721

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.

285. **EXCITONS IN SEMICONDUCTING SUPERLATTICES, QUANTUM WELLS, AND TERNARY ALLOYS**
M. D. Sturge, Department of Physics
(603) 646-2528 02-2 $100,000

Improve the understanding of optically excited states of quantum well and superlattice structures in semiconductors. Time-resolved tunable laser spectroscopy, with and without external perturbations such as magnetic field, electric field and uniaxial stress, will be employed to investigate exciton states in very short period superlattices where the "effective mass model" breaks down and electron-hole plasmas which form when the excitation density is high. Ternary alloys will be investigated to establish whether alloy disorder produces a mobility edge for excitons. Exciton-phonon coupling in II-VI compounds will also be examined.

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

286. **FUNDAMENTAL STUDIES OF NEW HIGH ENERGY PERMANENT MAGNET MATERIALS**
G. C. Hadjipanayis, Department of Physics
(302) 831-2661 02-2 $45,800

Investigation to advance the understanding of the magnetic properties of rare-earth-transition metal compounds and alloys, with the main thrust being to develop high performance permanent magnetic materials. Material phases considered are generally ternary or higher order compounds and alloys with unusually complex anisotropic structures. In some cases the rare-earth-transition metal materials are nitrogenated or carbonated to enhance their magnetic properties. Some sputtered thin film and multilayer phases are considered, and some new phases are reached by intermediate metastable phases formed by melt spinning. Materials investigated by comprehensive experimental techniques which include X-ray and neutron diffraction, electron microscopy, dc and ac magnetic susceptibility measurements, $Fe^{57}$ Mossbauer methods, and photoemission studies. Experimental results compared with first principles electronic structure calculations. Research performed in close collaboration with work at the University of Nebraska.

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

287. THEORETICAL STUDIES OF METALLIC ALLOYS
J. S. Faulkner, Department of Physics
(407) 367-3429 01-1 $96,628 from prior year

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), 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**

288. **HEAVY FERMIONS AND OTHER HIGHLY CORRELATED ELECTRON SYSTEMS**
P. U. Schlottmann, Department of Physics
(904) 644-0055 02-3 $37,243

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.

289. **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 high-resolution He-atom scattering to the investigation of surface dynamics of insulators, overlayers and crystal growth. Examples of ionic insulators studied include MgO, NiO, KCN, $Fe_2O_3$, $KTaO_3$, $BaTiO_3$, and $SrTiO_3$. Studies of ionic oxides during homo- and heteroepitaxial growth. Investigation of the dynamics of the head groups of alkyl thiols which self-assemble on gold and other, noble metals. Determination of surface magnetic properties of NiO and the superlattice $NiO/Fe_2O_3$, with exploratory study of $^3He$ scattering as a useful magnetic probe. Temperature dependent multiphonon measurements for some of the sample materials.

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

290. **QUANTUM-CONFINEMENT EFFECTS AND OPTICAL BEHAVIOR OF INTERMEDIATE SIZE SEMICONDUCTOR CLUSTERS**
J. H. Simmons, Department of Materials Science and Engineering
(904) 392-6679

P. H. Kumar, Department of Physics
(904) 392-6690 01-1 $134,802 (14 months)

Relationship between semiconductor microstructure, electronic band structure and linear and nonlinear optic properties of semiconductor cluster/glass composite; non-vanishing carrier wavefunctions at cluster surface, electronic band structure, enhanced carrier interactions with surface defects, carrier tunnelling in glass matrix. Nanosized semiconductor clusters (II-VI or III-V) isolated in glass matrix by sequential RF sputtering. Structural characterization with extraction TEM, electron and X-ray diffraction; role of exitons in quantum-confined clusters by optical absorption, photoluminescence, resonant Raman scattering, nonlinear optical band filling and pump-probe, including sub-picosecond spectral hole burning.

291. **X-RAY SCATTERING STUDIES OF NON-EQUILIBRIUM ORDERING PROCESSES**
S. E. Nagler, Department of Physics
(904) 392-8842 02-2 $60,000

X-ray and neutron scattering are being used to investigate the kinetics of first order phase transitions and elementary excitations in low dimensional quantum magnets. Time resolved scattering is used to measure, in real time, various model materials exibiting first order phase transitions that have been rapidly quenched through the transition by varying temperature or pressure. The coherence properties of synchrotron radiation are used to measure intensity-time autocorrelation functions. Magnetic excitations in chain materials with half integer spin and the effect of weak 3-D interactions are being investigated.

292. **STUDIES OF NOVEL SUPERCONDUCTORS**
G. R. Stewart, Department of Physics
(904) 392-9263/0521 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 measurements.

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

293. **FIRST-PRINCIPLES STUDIES OF PHASE STABILITY AND THE STRUCTURAL AND DYNAMICAL PROPERTIES OF METAL HYDRIDES**
M. -Y. Chou, Department of Physics
(404) 894-4688 02-2 $42,500 from prior year

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 method. 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.

294. **STRUCTURE AND DYNAMICS OF MATERIAL SURFACES, INTERPHASE-INTERFACES AND FINITE AGGREGATES**
U. Landman, School of Physics
(404) 894-3368 02-3 $186,200

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. Modelling uses molecular dynamical and quantum mechanical path-integral numerical methods.

295. **GROWTH, STRUCTURE AND STABILITY OF EPITAXIAL OVERLAYERS**
A. Zangwill, Department of Physics
(404) 894-7333 02-3 $65,000

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.

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

The phenomena 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 homopolymers.

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

297. **OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS**
W. M. Yen, Department of Physics and Astronomy
(706) 542-2491 02-2 $100,000

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**

298. **MEASUREMENTS OF CRYSTAL GROWTH KINETICS AT EXTREME DEVIATIONS FROM EQUILIBRIUM**
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.

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

Investigation of the properties of quantum gases of spin-polarized atomic hydrogen and deuterium. Attempt to reach sufficient densities and low temperatures that these unusual gases will undergo Bose-Einstein condensation using 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.

300. **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**

301. **DIFFRACTION STUDIES OF THE STRUCTURES OF GLASSES AND LIQUIDS**
S. C. Moss, Department of Physics
(713) 743-3539 02-1 $105,600

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 with 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**

302. **SEGMENTAL INTERPENETRATION AT POLYMER-POLYMER INTERFACES**
T. P. Russell, Almaden Research Center
(408) 927-1638 03-2 $112,251

The behavior of block copolymers at interfaces will be studied with the use of neutron and X-ray reflectivity, XPS, DSIMS, and FRES. The subjects of investigation will include the behavior of diblock copolymer in confined geometries, the interfacial behavior of 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**

303. **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. The experimental method employed is high-resolution electron energy loss spectroscopy (EELS) with an energy resolution of 3-5 meV. Detailed surface phonon dispersion information is to be obtained on copper, silver, iron, iron/silver and aluminum/silicon with and without adsorbates such as hydrogen, oxygen, and sulfur. Results are to be compared with realistic theoretical models of surface lattice dynamics and inelastic electron scattering.

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

304. **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 gas phase species concentration with these processes and resultant particle sizes. Absorption and other spectroscopic methods utilized to follow gas phase species concentrations. Materials studies include silica, titania, alumina and germania.

305. **DE-ALLOYING AND 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

Two major areas of focus are: (1) alloy corrosion and the roughening transition and (2) the role of selective dissolution in the stress corrosion cracking of alloy systems. Alloy corrosion processes are studied on Ag-Au and Cu-Au using electrochemical techniques, in-situ scanning tunneling microscopy (STM), and X-ray scattering and reflectivity. The STM and X-ray work address the roughening transition known to occur in alloy systems undergoing corrosion at electrochemical potentials greater than the "critical potential." Molecular dynamic and Monte Carlo simulation techniques are being used to examine various aspects of the roughening transition.

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

306. **ANALYTICAL ELECTRON MICROSCOPY OF BIMETALLIC CATALYSTS**
C. E. Lyman, Department of Metallurgy and Materials Engineering
(215) 758-4220 01-1 $87,425

Elucidation of structure-property relationships in platinum-rhodium bimetallic catalyst for $NO_x$ 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 $NO_x$ in hydrogen.

307. **HIGH RESOLUTION MICROSTRUCTURAL AND MICROCHEMICAL ANALYSIS OF ZIRCONIA EUTECTIC INTERFACES**
M. R. Notis, Department of Materials Science and Engineering
(215) 758-4225 01-1 $102,212

Eutectic interfaces studied in as-grown $MnO-ZrO_2$, $NiO-ZrO_2(Y^{20}3$ $CoO-ZRO_2(CaO)$, 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.

308. **STRUCTURAL PHASE TRANSITIONS IN MIXED SYSTEMS**
J. Toulouse, Department of Physics
(215) 758-3960 01-1 $52,061

Competing structural phase transitions and phase transitions driven by competing interactions in mixed systems. Ferro-antiferro competition in mixed fluoroperovskites; $Rb_{1-x}K_xCaF_3$, R point vs. M point in the brillouin zone, effect of Rb substitution on softening of at R point (antiferrodistortive coupling); $Rb_{1-x}K_xZnF_3$, point vs. R. point in the Brillouin zone, competition between zone center (ferroelectric) and zone boundary mode; dielectric, ultrasonic, Raman scattering and neutron scattering techniques. Nonlinear elastic effects in mixed oxyperovskites; $K_{1-y}Li_yTaO_3$ and $NTa_{1-x}Nb_xO_3$, dielectric and elastic effects, third-order elastic constants, interplay between polar precursor clusters and nonlinear elastic effects. Martensitic phase transitions and comparison with paraelectric effects in highly polarizable crystals; nonlinear responses to external fields; $Ni_xAl_{1-x}$, precursor clusters and anharmonicity, elastic nonlinearities in second and third order elastic constants, resistivity measurements.

309. **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 from prior year

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.

310. **ROLE OF PHYSICAL STRUCTURE IN ION MOVEMENT IN GLASSES**
H. Jain, Department of Materials Science and Engineering
(215) 758-4217 01-3 $105,600 (24 months)

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**

311. **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 $0 (0 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 embedding of zeolites work 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 NaC1 and $CaF^2$ clusters, and sputtering of solid C by $H^2O$ clusters.

## UNIVERSITY OF MAINE
**5764 Sawyer Research Center**
**Orono, ME 04469**

312. **STRUCTURAL, ELECTRONIC AND CHEMICAL PROPERTIES 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, Ti, Cu, Mg0, $Y_2O_3$, and $SiO_2$) on single crystal $Al_2O_3$ 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 Ave.**
**Cambridge, MA 02139**

313. **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 $455,000

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.

314. **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 from prior year

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.

315. **SLIP TWINNING AND TRANSFORMATION IN LAVES PHASES**

S. M. Allen, Department of Materials Science and Engineering
(617) 253-6939

J. D. Livingston, Department of Materials Science and Engineering
(617) 253-0059 01-2 $100,572

Demonstrate that a variety of room-temperature deformation processes possible in Laves phases. Two methods to enhance plastic deformation. First, deformation in alloys in which the Laves phase exists as discrete second-phase particles in a solid-solution matrix. Second, microhardness indentations to produce localized deformation (with a significant triaxial component to the loading), and to prepare high-quality thin-foil specimens for examination in the transmission electron microscope.

316. **GRAIN BOUNDARIES IN COMPLEX OXIDES**

Y-M. Chiang, Department of Materials Science and Engineering
(617) 253-6471 01-2 $145,444

Complex lattice defect structures, ionic space charge effects at grain boundaries; $TiO_2$ with trivalent and pentavalent cation dopants; quantitative comparison between space charge theory and grain boundary segregation; defect formation energies at grain boundaries and their variation from boundary to boundary; quantitative determination of grain boundary accumulation of dopants by STEM. Determination of grain boundary thermodynamic properties and size-dependent segregation and transport phenomena in nanocrystalline $TiO_2$; effect of solute segregation on grain boundary thermodynamics and kinetic properties; effects of space charge on grain growth and deformation.

317. **FATIGUE FRACTURE AT INTERFACES: MICROMECHANICS AND APPLICATIONS TO COATED MATERIALS**

S. Suresh, Department of Materials Science and Engineering
(617) 253-3233 01-2 $108,570

Experimental and numerical investigation of fatigue at interfaces; evolution of cyclic near-tip fields for fatigue cracks along or normal to interfaces; conditions for growth or deceleration/arrest of fatigue cracks approaching an interface at an arbitrary angle; effects of variable amplitude loads with tensile overloads on near-tip fields and crack growth; micromechanisms of near-interface deformation; numerical simulation of cyclic near-tip fields arising from temperature fluctuations, mechanical load fluctuations, and thermomechanical loads for flaws along or at arbitrary angles to interfaces, model parametric studies of fatigue cracking of coated materials with and without interlayers.

318. **OXIDES AND SURFACE MAGNETISM**

R. C. O'Handley, Department of Materials Science and Engineering
(617) 253-6913

M. Oliveria, Department of Materials Science and Engineering
(617) 258-6113 01-3 $110,000

Study of surface magnetism in metal-oxide systems and the development of novel magnetic composites. Research will focus on magnetic properties at free surfaces and interfaces. Surface characterization techniques will be utilized to understand the chemical (AES and Auger polar intensity plots), structural (LEED), and magnetic properties (secondary electron spin polarization analysis and magneto-optic Kerr effect) of the surfaces and interfaces. Novel composite development will focus on both 3-D and planar multilayer structures.

319. **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.

320. **OXIDATION OF METALS AND ALLOYS WITH EMPHASIS ON SUPERCONDUCTING OXIDES**
J. B. Vander Sande, Department of Materials Science and Engineering
(617) 253-6933 01-3 $164,502

Kinetics of superconducting oxide formation from metallic alloys subjected to oxidation; textured microstructures arising from solid state reactions in temperature gradients; high magnetic fields to induce texture in superconducting oxide/silver composites; improvement in the texture and critical current density of superconducting oxide/silver microcomposites through mechanical deformation.

321. **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 crystalline 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.

322. **MICROSTRUCTURAL DESIGN IN CLEEULAR MATERIALS**
L. J. Gibson, Department of Civil Engineering
(617) 253-7107 01-5 $83,074

Investigation of efficient microstructures for cellular solids through micromechanical modelling 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 with the proposed microstructures.

323. **IDENTIFICATION OF NITRIDING MECHANISMS IN HIGH PURITY REACTION BONDED SILICON NITRIDE**
J. Haggerty, Materials Processing Center
(617) 253-2129 01-5 $0 from prior year

Experimental and process modelling of silicon nitridation kinetics in sintering of reaction bonded silicon nitride. In house preparation and characterization of laser synthesized silicon powders with low oxygen content. Investigation of effects of surface Si-H bonds on early stage nitridation, of mechanism of formation amorphous nitride layer and of nucleation and heteroepitaxial growth of crystalline silicon nitride grains on silicon particles. Treatment of silicon powder surface, coatings, atmosphere, grain-size/particle size ratio, and other factors influencing nucleation rate will be investigated. Transition from fast to slow reaction stages will be investigated.

324. **SYSTEMATIC GLOBAL RENORMALIZATION-GROUP STUDIES OF DETAILED MODELS FOR CONDENSED MATTER SYSTEMS**
A. N. Berker, Department of Physics
(617) 253-2176 02-3 $43,999

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.

325. **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) 258-3810 03-2 $46,750 (0 months)

Construct a special purpose small angle neutron scattering diffractometer at the Intense Pulsed Neutron Source (IPNS) of Argonne National Laboratory. 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**

326. **MAGNETIC MULTILAYER PHYSICS**
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. Develop and use a variable temperature torque magnetometer to measure dc multilayer anisotropy and magnetization. Model the effects of magnetization gradients and interface frustration on interface anisotropy.

## MICHIGAN STATE UNIVERSITY
**East Lansing, MI 48824**

327. **HIGH TEMPERATURE STABILITY, INTERFACE BONDING, AND MECHANICAL BEHAVIOR IN B-NIAL AND $NI_3AL$ MATRIX COMPOSITES WITH REINFORCEMENTS MODIFIED BY ION BEAM ENHANCED DEPOSITION**
D. S. Grummon, Department of Metallurgy, Mechanics, and Materials Science
(517) 353-4688 01-2 $61,600

The microstructural stability and mechanical properties of reinforced ordered intermetallics (primarily B-NiAl) by $Al_2O_3$ and SiC, particles, whiskers, and short fibers. Interfacial bonding has been modified by an alumina coatings applied by ion beam enhanced deposition. High-temperature strength and low-temperature toughness will be measured.

328. **DISORDER AND FAILURE: SELECTED APPLICATIONS TO BRITTLE FRACTURE, CRITICAL CURRENT AND DIELECTRIC BREAKDOWN**
P. M. Duxbury, Department of Physics and Astronomy
(517) 353-9179 01-3 $66,560

Development of generic models for electrical, dielectric, mechanical and superconducting failure; analytic expressions for size effect, failure distribution, and crossover from nucleation stage to catastrophic failure stage. Disorder and failure in random composites; effect of microstructural disorder on failure of composites; scaling behavior of damage nucleation, damage localization and catastrophic failure in random composites; fracture of interpenetrating phase composites; analytic and numeric analysis of defect shapes and damage nucleation. Activated and diffusion limited damage nucleation; development of scaling theories for time to failure and its statistics for subcritical crack growth in random systems as function of disorder, system size, and temperature. Atomic defects and brittle failure of graphite sheets containing random defects. Effective elastic and failure properties of cellular materials as function of porosity, disorder and sample size; ductile and brittle ligament response. Critical current as function of crack length, pinning strength and vortex density for superconductors; cross-over from flux flow channel limit to collective pinning limit; vortex configuration in a superconducting diode. Extension of dielectric breakdown model to include space charge and environmental effects, diffusion limited and activated processes, and critical local field.

## MICHIGAN TECHNOLOGICAL UNIVERSITY
**1400 Townsend Drive**
**Houghton, MI 49931**

329. **BOUNDARY STABILITY UNDER NONEQUILIBRIUM CONDITIONS**
S. Hackney, Metallurgical and Materials Engineering Department
(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. Surface and thin film instabilities.

## UNIVERSITY OF MICHIGAN
**Ann Arbor, MI 48109-2136**

330. **SOLUTE EFFECTS ON OXIDE CERAMICS AND THEIR GRAIN BOUNDARIES**
I-W. Chen, Department of Materials Science and Engineering
(313) 763-6661 01-2 $144,165

Solute-defect interactions and segregation; $CeO_2$, $Y_2O_3$ and $ZrO_2$ host oxides; solid solutions with oxides of divalent Mg, Ca, and Sr, trivalent Sc, Yb, Y, Gd, and La, tetravalent Ti and Zr, and pentavalent Nb and Ta. Static grain growth, dynamic grain growth and related mechanical phenomena; mechanisms for solute drag, solute-defect interactions; static grain growth experiments, grain boundary mobility, compression tests, dislocation creep; construction of stress-strain constitutive relation incorporating grain growth; microstructural and microchemical characterization. Densification kinetics, microstructure development, grain boundary mobility; doped solid solutions; effect of solute drag on sintering of second phase ceramics; effect of initial porosity. Electrical conductivity, space charge effects; ac impedance spectroscopy.

331. **THE ROLE OF GRAIN BOUNDARY CHEMISTRY AND STRUCTURE IN THE ENVIRONMENTALLY-ASSISTED INTERGRANULAR CRACKING OF NICKEL-BASE ALLOYS**
G. S. Was, Department of Nuclear Engineering
(313) 763-4675 01-2 $139,224

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).

332. **THE STRUCTURAL BASIS FOR FATIGUE FAILURE 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.

333. **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.

334. **SYNCHROTRON STUDIES OF NARROW BAND MATERIALS**
J. W. Allen, Department of Physics
(313) 763-1150 02-2 $90,000

Conduct a program of spectroscopic studies of the electronic structure of narrow band actinide, rare-earth and transition metal materials, emphasizing the use of synchrotron radiation but including 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 transition metal oxide materials, including insulator-metal transitions in each of these, and high temperature superconductivity in the latter. The data is analyzed using density-functional calculations and many-body Hamiltonian models.

**335. GROWTH AND NONLINEARITY**
L. M. Sander, Department of Physics
(313) 764-4471

R. Savit, Department of Physics
(313) 764-3426 02-3 $104,984

Theoretical proposal at the forefront of a recent approach to understanding the relationships between growth mechanisms, structure, and properties of nonequilibrium systems, such as smoke, colloids, deposition of vapors and electrolytes, which have been shown to give rise to scale invariant fractal-like structures. Objects of this type have a morphology which lies between conventionally studied crystalline geometry 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 helping scientists understand the dynamics of such random scale-invariant objects. The principal investigators expect to rely heavily on both analytical techniques and numerical simulations in this work.

## UNIVERSITY OF MINNESOTA
**Minneapolis, MN 55455**

**336. CRYSTALLINE-AMORPHOUS INTERFACES AND AMORPHOUS FILMS IN GRAIN BOUNDARIES**
C. B. Carter, Department of Chemical Engineering and Materials Science
(612) 625-8805 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 $SiO_2$ and CaO vapor for investigations of grooving, film penetration and dewetting.

**337. 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 $62,496

A study of the micromechanics of small volumes with the aim of understanding brittle fracture in both bulk single crystals and polycrystals as well as at thin film interfaces. Au, Fe, and Ta films constrained by brittle substraits. Theoretical approaches are finite element, embedded atom, and discretized dislocation; experimental techniques include SEM, TEM, STM, AFM and continuous nanoindentation and microscratch.

**338. THEORETICAL STUDY OF REACTIONS AT THE ELECTRODE-ELECTROLYTE INTERFACE**
J. W. Halley, Department of Physics and Astronomy
(612) 624-0395 01-3 $85,217 (14 months)

Electron transfer rates predicted by numerical methods. Molecular dynamics used to describe solvent dynamics and equation of motion methods to obtain the electronic structure of disordered oxides. Emphasis on electron transfer involving ions known to be important in enhancing stress corrosion cracking in light water reactors and on calculation of the rates of electron transfer at oxide surfaces. Program involves collaboration with Argonne National Laboratory.

**339. A STUDY OF SCALE CRACKING AND ITS EFFECTS ON OXIDATION**
D. A. Shores, Department of Chemical Engineering and Materials Science
(612) 625-0014 01-3 $153,058

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

340. **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 from prior year

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.

341. **THEORY OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF SOLID STATE OXIDES**
J. R. Chelikowsky, Department of Chemical Engineering and Materials Science
(612) 625-4837 02-3 $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**

342. **HIGH PRESSURE OPTICAL STUDIES OF SEMICONDUCTORS AND HETEROSTRUCTURES**
H. R. Chandrasekhar, Department of Physics and Astronomy
(314) 882-6086 02-2 $50,000 from prior year

Investigation of the electronic structure, intrinsic and extrinsic, of semiconductors and heterostructures which exhibit electro-optical and magneto-optical properties, using high pressure diamond anvil cell at cryogenic temperatures to tune such properties in a controlled manner. Spectroscopic techniques include photoluminescence, photoreflectance, Raman scattering and excitation spectroscopy. Energies and pressure coefficients of various band extreme 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.

343. **INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION**
W. B. Yelon, Department of Physics
(314) 882-5236 02-2 $30,000

This project aims at the development and use of ultra high intensity Mossbauer sources for scattering experiments. The techniques 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 constructed 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.

## UNIVERSITY OF MISSOURI AT KANSAS CITY
**Kansas City, MO 64110-2499**

344. **THEORETICAL STUDIES ON THE ELECTRONIC STRUCTURES AND PROPERTIES OF COMPLEX CERAMIC CRYSTALS AND NOVEL MATERIALS**
W-Y. Ching, Department of Physics
(816) 235-2503 01-1 $102,903

Calculation by means of orthogonalized linear combination of atomic orbitals (OLCAO) of electronic structure and linear optical properties and defect properties for a large number of oxide, nitride, phosphate, silicate, III-V semiconductors, metallic glass and high-$T_c$ superconducting materials. Local density functional 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. Properties of fullerenes.

## UNIVERSITY OF MISSOURI AT ROLLA
**278 McNutt Hall**
**Rolla, MO 65401**

345. **CHARACTERIZATION OF ELECTRICALLY CONDUCTING OXIDES**
H. U. Anderson, Department of Ceramic Engineering
(314) 341-4886 01-3 $99,704

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**

346. **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 deutreated samples and optical studies involving birefringence, small angle light scattering, and Brillouin scattering to measure degree of chain alignment and sound velocity and attenuation as affected by polymer processing and by temperature and pressure induced phase transitions including theoretical studies of crystal elastic energy and statistical mechanics of linear polymers.

## UNIVERSITY OF NEBRASKA
**Lincoln, NE 68588-0113**

347. **FUNDAMENTAL STUDIES OF NEW HIGH-ENERGY PERMANENT MAGNET MATERIALS**
D. J. Sellmyer, Department of Physics
(402) 472-2407 02-2 $75,000

Investigations to advance the understanding of the magnetic properties of rare earth - transition metal compounds and alloys, with the main thrust being to develop high performance permanent magnetic materials. Material phases considered are generally ternary or higher order compounds and alloys with unusually complex anisotropic structures. In some cases the rare-earth-transition metal materials are nitrogenated or carbonated to enhance their magnetic properties. Some sputtered thin film and multilayer phases are considered, and some new phases are reached by intermediate metastable phases formed by melt spinning. Materials investigated by comprehensive experimental techniques which include X-ray and neutron diffraction, electron microscopy, dc and ac magnetic susceptibility measurements, $Fe_{57}$ Mossbauer methods, and photoemission studies. Experimental results compared with first principles electronic structure calculations. Research performed in close collaboration with work at the University of Delaware.

## UNIVERSITY OF NEVADA
**Reno, NV 89557**

348. **PHOTOPHYSICAL PROPERTIES OF TRIPLET EXCITATIONS ON POLYMERIC SYSTEMS**
R. D. Burkhart, Department of Chemistry
(702) 784-6041 03-1 $106,250 from prior year

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**

349. **EFFECTS OF FRACTURE SURFACE INTERFERENCE ON SHEAR CRACK GROWTH**
T. S. Gross, Department of Mechanical Engineering
(603) 862-2445 01-2 $66,481 (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, nonlinear 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**

350. **RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE SILICATES, COMPLEX OXIDES, AND PHOSPHATES**
R. C. Ewing, Department of Geology
(505) 277-4163 01-1 $78,081 from prior year

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 ($UO_2$).

351. **PARTICLE-INDUCED AMORPHIZATION OF CRYSTALLINE SILICATES, COMPLEX OXIDES AND PHOSPHATES**
R.C. Ewing, Department of Geology
(505) 277-4163 01-1 $108,081

Investigation of irradiation effects on transition from crystalline to aperiodic state in naturally occurring materials (complex oxides, silicates and phosphates) and ion-irradiated ceramics; effects of structure and bonding, cascade energy, defect accumulation and temperature on the amorphization of complex ceramic materials; structural types include zircon ($AB0_4$), olivine, garnet, aluminosilicates, pyrochlore. Techniques include X-ray diffraction, high-resolution transmission electron microscopy (HRTEM), extended x-ray absorption fine-structure (EXAFS) and near-edge spectroscopy (XANES).

352. **ADSORPTION STUDIES AT A SOLID-LIQUID INTERFACE**
J. A. Panitz, Department of Physics
(505) 277-8488 01-1 $107,408

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**

353. **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.

354. **LOCALIZED FRACTURE DAMAGE EFFECTS 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.

355. **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) 515-3482    02-2 $340,000

Development, improvement, and operation of beamlines X-11A and B at the National Synchrotron Light Source, Brookhaven National Laboratory. Transmission, fluorescence electron-yield, diffraction anomalous fine structure 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.

356. **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.

357. **THEORETICAL STUDIES OF SURFACE REACTIONS ON METALS AND ELECTRONIC MATERIALS**
J. L. Whitten, Department of Chemistry
(919) 515-7277    03-1 $105,000 (14 months)

Theoretical investigations of the structure and reactivity of small molecules adsorbed on transition metal and semiconductor substrates. Development and application of theoretical techniques that will provide a molecular level of fundamental understanding for surface processes, especially reaction mechanisms, energetics and adsorbate atomic and electronic structure. Electronic structures obtained by an ab initio embedding formalism that permits an accurate determination of reaction energetics and adsorbates. Major applications treated are for reactions on surfaces of silicon, carbon, nickel, and ruthenium.

## UNIVERSITY OF NORTH CAROLINA
**Chapel Hill, NC 27599**

358. **SOLID-STATE VOLTAMMETRY AND SENSORS IN GASES AND OTHER NONIONIC MEDIA**
R. Murray, Department of Chemistry
(919) 962-6296    03-2 $42,500

Miniaturized electrochemical cells based on the use of microdisk, microband, and interdigitated array electrodes have been employed in a program aimed at developing a range of electrochemical methodologies suitable for quantitative voltammetry of electroactive solutes dissolved in solid and semisolid polymeric solvents. Potential sweep, step, and ac microelectrode voltammetries have been evaluated and adapted to measurement of exceedingly slow transport of electroactive solutes, with particular application to transport phenomena in poly(ether) "polymer electrolyte" solvents. Transport rates of dissolved electron transfer donors and acceptors are studied as a function of polymer MW, phase-state, small molecule plasticization, temperature, electrolyte concentration, and of the equivalent charge transport by electron self exchanges between dissolved donor-acceptor pairs. Methods are also being developed for measurement of electron transfer dynamics in polymer solvents with attention to slow solvent dipole/solvent dynamics control of electron transfer rates and to diffusion-rate dependent distances-of-electron transfer as would occur when diffusion is very slow. These first quantitative voltammetric measurements in solid and semisolid state phases are aimed at developing a capacity for fundamental, quantitative studies of solid-state charge and mass transport phenomena and at their exploitation for solid-state analysis.

## UNIVERSITY OF NORTH TEXAS
**P.O. Box 5308**
**Denton, TX 76203**

359. **IMPURITY-INDUCED CORROSION AT GRAIN BOUNDARIES, METAL-OXIDE INTERFACES AND OXIDE SCALES**
J. A. Kelber, Center for Materials Characterization
(817) 565-3265 01-3 $150,000 (18 months)

Obtain a fundamental understanding concerning the effects of sulphur and other electronegative adsorbates on interfacial chemistry and topography, and how such effects can be counteracted by the use of other, selected, dopants. Interfaces of interest are grain boundaries, oxide and metal free surfaces, and oxide/metal internal surfaces.

## NORTHEASTERN UNIVERSITY
**110 Forsyth Street**
**Boston, MA 02115**

360. **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**

361. **ATOMIC RESOLUTION ANALYTICAL ELECTRON MICROSCOPY OF GRAIN BOUNDARY PHENOMENA ASSOCIATED WITH ISOLATED-SINGLE GRAIN BOUNDARIES IN BICRYSTALS OF $SRTIO_3$**
V. P. Dravid, Department of Materials Science and Engineering
(708) 467-1363 01-1 $133,000 from prior year

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.

362. **STRUCTURE-PROPERTY RELATIONSHIPS IN HIGHLY DEFECTIVE OXIDES**
T. O. Mason and J. B. Cohen, Department of Materials Science and Engineering
(708) 491-3198

D. E. Ellis, Department of Physics and Astronomy
(708) 491-3665 01-1 $249,967

Study of defect clustering, interfaces, and related properties of oxides involving transport and nonstoichiometry measurements, diffraction, and quantum theoretical methods. Oxides of interest include highly defective transition metal monoxides (FeO, MnO, CoO, NiO) and rare earth, alkaline earth cuprates, including high-$T_c$ superconductors. In situ measurements within a high pressure oxygen cell to study higher defect concentrations. Structural and valence studies by diffuse X-ray scattering, neutron diffraction, 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. Modelling of defect dependent properties of materials.

363. **ATOMIC STRUCTURES AND COMPOSITIONS OF INTERNAL INTERFACES**
D. N. Seidman, Department of Materials Science and Engineering
(708) 491-4391 01-1 $149,833

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.

364. **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 modelling 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.

365. **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 $81,602

Investigation of the fundamentals of mechanical behavior of nanocrystalline iron and steel. The influence of decreasing grain size and of interstitial content on 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 in interpreting results of mechanical measurements.

366. **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

Diamond nucleation and growth on carbide and noncarbide surfaces; mechanisms of nucleation; interface properties. Diamond nucleation on fullerenes; ion activation, effects of ion energy, mass and ion type; preparation of large fullerene and buckytube substrates; in situ characterization of diamond nucleation and growth using scanning ellipsometry, Raman scattering and Auger/ESCA measurements. Growth of copper, nickel, and copper/nickel on single crystal diamond to attempt formation of epitaxial layer; epitaxial metal layers characterized by Rutherford backscattering/ channeling and HREM; selective area epitaxy of copper on diamond and overgrowth of diamond. Growth of diamond on amorphous carbon, SiC, c-BN, $Si_3N_4$ and $C_xN_y$ films; role of graphitic carbon; role of noncarbon surfaces; in situ characterization by Auger, ESCA, Raman and HREED; modelling of nucleation and growth.

367. **DEFECT STRUCTURE OF SEMICONDUCTING AND EPITAXIAL INSULATING OXIDES**
B. W. Wessels, Department of Materials Sciences and Engineering
(708) 491-3219 01-3 $70,380

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.

368. **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.

369. **RELATIONSHIPS BETWEEN MICROSTRUCTURE AND CREEP AND SHRINKAGE OF CEMENT**
H. Jennings, Department of Civil Engineering
(708) 491-4858 01-5 $87,780

Study of the effect of moisture on the microstructure of cement. Early age "floc" structure of fresh paste and its relationship to the structure of mature pastes. Influence of moisture and other environmental variables including temperature on the microstructure at all ages. Effect of applied load on microstructure. Mechanical properties of cement.

370. **ENERGETICS, BONDING MECHANISM AND ELECTRONIC STRUCTURE OF METAL/CERAMIC INTERFACES**
A. J. Freeman, Department of Physics and Astronomy
(708) 491-3343 02-3 $79,990

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 $VO_2/TiO_2$ interfaces.

371. **MIXED IONIC AND ELECTRONIC CONDUCTIVITY IN POLYMERS**
M. A. Ratner, Department of Chemistry
(708) 491-5652

D. E. Shriver, Department of Chemistry
(708) 491-5655 03-2 $94,000

This proposal is an investigation of ionic transport along and through interfaces, both within a given solid electrode or electrolyte and between solid electrodes and electrolytes. The objective is mechanistic understanding of which processes result in overpotential, degradation, charge accumulation, and enhanced mobility at such interfaces. Two general classes of materials will be investigated: siloxane based polymer electrolytes, and layered chalcogenide 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.

372. **STRUCTURE AND SHEAR RESPONSE OF LIPID MONOLAYERS**
P. Dutta, Department of Physics and Astronomy
(708) 491-5465

J. B. Ketterson, Department of Physics and Astronomy
(708) 491-5468 03-3 $52,500 (6 months)

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 fluorescence 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**

373. **SINGLE-ELECTRON TUNNELING**
S. T. Ruggiero, Department of Physics
(219) 631-7463 02-2 $49,000

Charging effects in ultra-small-capacitance metal particles will be studied by electron tunneling, using multiple-barrier tunnel structures of the form metal/barrier/particles/barrier/metal, where the particles are 1-1000 nm 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**

374. **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 from prior year

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.

375. **REALISTIC THEORIES OF HEAVY ELECTRON AND OTHER STRONGLY CORRELATED MATERIALS**
D. Cox, Department of Physics
(614) 292-0620 02-3 $60,000 (11 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.

376. **STRONGLY INTERACTING FERMION SYSTEMS**
J. W. Wilkins, Department of Physics
(614) 292-5193 02-3 $130,000

Development of new methods for 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 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.

377. **NEW CARBOHYDRATE-BASED MATERIALS**
M. R. Callstrom, Department of Chemistry
(614) 292-0917 03-1 $70,000

Synthesis of novel polymeric materials designed to incorporate many of the useful properties and functionality of natural polysaccharides. The approach is to use carbohydrates as templates for the introduction of polymerizable side-groups. The synthetic methodology involves both enzymatic and chemical synthesis techniques to prepare selectively functionalized monomers followed by chemical polymerization. The introduction of charged, hydrophobic, and other desired functionality to these carbohydrate-based polymers will provide synthetic control of polymer properties and a better understanding of the relation of functionality to properties. These materials will be investigated for a) the stabilization of enzymes and b) the preparation of functional hydrogels.

378. **MOLECULAR/POLYMERIC MAGNETISM**
A. J. Epstein, Department of Physics
(614) 292-1133/3704 03-1 $148,266 (9 months)

Study of cooperative magnetic behavior and its microscopic origins in molecular and polymeric materials. Synthesis and characterization of novel ferromagnets and elucidation of the origins of ferromagnetic exchange. Objective is to develop design criteria for the synthesis of new ferromagnetic materials possessing desirable physical properties including high temperature transitions to a ferromagnetic state. Study of magnetism in molecular ferromagnets and origins of the ferromagnetic exchange. Synthesis of $V(TCNE)_x^y$ (solvent), including single crystals, and analogous molecular-based organic systems. Measurements of magnetism as a function of field, temperature, and pressure and comparison of results with models of one-dimensional ferro-ferrimagnetism. X-ray and inelastic neutron scattering measurements for magnetic structure.

## OHIO UNIVERSITY
**Athens, OH 45701-2979**

379. **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**

380. **RHEO-OPTICAL STUDIES OF MODEL "HARD SPHERE" SUSPENSIONS**
B. J. Ackerson, Physics Department
(405) 744-5819 01-3 $55,532

Spontaneous and artificially 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.

## OLD DOMINION UNIVERSITY
**Norfolk, VA 23529**

381. **DYNAMICS OF SURFACE MELTING**
H. E. Elsayed-Ali, Department of Electrical and Computer Engineering
(804) 683-3741 03-3 $146,000 (14 months)

Experimental investigation of the dynamics of surface melting for metallic single crystals and thin epitaxial metal films. Time-resolved reflection high energy electron diffraction (RHEED), with picosecond time resolution, is used to study the surface melting upon fast heating and cooling. Observation of the time evolution of lattice expansion during ultrafast heating. Studies of the role of surface roughness on the nucleation and the growth of disorder during surface melting. Examples of systems investigated are surfaces of Pb and Bi, and expitaxial films of Pb on Si.

## OREGON STATE UNIVERSITY
**Corvallis, OR 97331**

382. **HYPERFINE EXPERIMENTAL INVESTIGATIONS OF POINT DEFECTS AND MICROSCOPIC STRUCTURE IN COMPOUNDS**
J. A. Gardner, Department of Physics
(503) 737-3278 01-1 $115,000

Perturbed angular correlation (PAC) spectroscopy of nuclear gamma rays to investigate defect complexes, and microscopic structure in ceria, zirconia, and II-VI compounds containing either 111-In or 181-Hf as a probe. PAC characterizations of free energies, transformation mechanisms, equilibrium phase boundaries, diffusion and relaxation models, short range order, order-disorder reactions, and elevated-temperature/time dependent effects. NMR and EXAFS measurements to complement and expand the studies of local structure and oxygen vacancy dynamics.

383. **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 97403-1274**

384. **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 and, when available, at the Advanced Light Source. Metals investigated include mainly the 4d and 5d transition metals, and both electropositive and electronegative adsorbates are considered. Emphasis is on determination of electronic structure for intrinsic surface states and resonances, and in particular, when desirable, a complete mapping of the two-dimensional Fermi contours associated with the electron states. Attempts made to relate the observed details of the electronic structure to other properties of the surface systems.

385. **MONITORING INTERFACIAL DYNAMICS BY PULSED LASER TECHNIQUES**
G. L. Richmond, Department of Chemistry
(503) 346-4635 03-2 $0 (0 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
**104 Davey Laboratory**
**University Park, PA 16802**

386. **VIBRATIONAL AND ELECTRONIC PROPERTIES OF FULLERENE AND CARBON-BASED CLUSTERS**
J. S. Lannin, Department of Physics
(814) 865-9231 01-1 $102,430

Raman scattering studies of $A_xC_{60}$ and $A_xB_{1-x}C_{60}$ (where A = Rb, K, Li, and Na) thin and ultrathin films to clarify effects of alkali type and concentration on structural disorder and electron-phonon coupling. Metal-$C_{60}$ interactions. Role of additional charge transfer in electron-phonon coupling effects. Study of $Ba_xC_{60}$ ultrathin films with IERS. Studies using IERS on ultrathin films of metal species incorporated into multilayer structures. Determination if low frequency phonons play a significant role in electron-phonon coupling and superconductivity. Examination of other fullerene systems.

387. **DESIGN, PROCESSING AND MECHANICAL BEHAVIOR OF LAMINATED CERAMIC COMPOSITES**
D. J. Green, Department of Materials Science and Engineering
(814) 863-2011 01-2 $30,000

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 gage techniques.

388. **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.

389. **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 from prior year

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.

390. **PARTITION OF NITROGEN, OXYGEN AND HYDROGEN BETWEEN THE WELD POOL AND ITS ENVIRONMENT**
T. DebRoy, Department of Materials Science and Engineering
(814) 865-1974  01-5 $160,015

Improved control of weld metal composition and properties through fundamental understanding of welding. Partition of nitrogen, oxygen and hydrogen in weld pool and its environment. Understanding principles of partition through physical simulation. Improved understanding of the role of oxygen in affecting the dynamics of heat transfer and fluid flow. Incorporation of improved interfacial physics and chemistry in numerical simulation of weld pool behavior. Ongoing collaborative program with Oak Ridge National Laboratory.

391. **AN INVESTIGATION OF THE STRUCTURE AND PHASE RELATIONS OF C-S-H GELS**
M. W. Grutzeck,
(814) 863-2779  01-5 $90,347 (14 months)

Structural and compositional evolution of calcium silicate and calcium silicate hydrates (C-S-H) gels during hydration; magic angle spinning and cross polarization magic angle spinning NMR, TEM, trimethylsilylation, BET, SEM, XRD and TGA/DTA; effect of drying methods, alkali chloride and carbonation on C-S-H structure. Hydration model developed.

392. **MULTIFUNCTIONAL NANOCOMPOSITE MATERIALS**
R. Roy, Materials Research Laboratory
(814) 865-3421

S. Komarneni, Materials Research Laboratory
(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
**3231 Walnut Street**
**Philadelphia, PA 19104**

393. **SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY OF CERAMIC GRAIN BOUNDARIES**
D. A. Bonnell, Department of Materials Science and Engineering
(215) 898-6231  01-1 $108,000

Investigation of the effects of interfacial structure and chemistry on the local electrical properties at grain boundaries in ceramics using scanning tunneling microscopy (STM) and transmission electron microscopy (TEM). Develop improved understanding regarding the imaging of large band gap structures in STM. Studies to include doped and undoped, single crystal and polycrystalline Si, ZnO, $TiO_2$, and $SrTiO_3$.

394. **STRUCTURE AND DYNAMICS IN LOW-DIMENSIONAL GUEST-HOST SOLIDS**
J. E. Fischer, Department 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.

395. **ATOMISTIC STUDIES OF GRAIN BOUNDARIES AND HETEROPHASE INTERFACES IN ALLOYS AND COMPOUNDS**
V. Vitek, Department of Materials Science and Engineering
(215) 898-6703  01-1 $112,983

Atomistic computer simulation studies of grain boundaries in binary ordered and disordered alloys. Investigation of grain boundaries with segregated solutes. Study of grain boundary and metal-ceramic interface electronic structure. Methods of calculation of interatomic forces. $Ni_3Al$, $Ti_3Al$, TiAl, Cu-Bi and Cu-Ag are candidate alloys to be studied.

396. **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.

397. **CONDENSED MATTER PHYSICS AT SURFACES AND INTERFACES OF SOLIDS**
E. J. Mele, Department of Physics
(215) 898-3135 02-3 $55,000

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**

398. **THE RELATIONSHIP BETWEEN MICROSTRUCTURE AND MAGNETIC PROPERTIES IN HIGH-ENERGY PERMANENT MAGNETS CHARACTERIZED BY POLYTWINNED STRUCTURES**
W. A. Soffa, Department of Materials Science 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. An APB pinning model will be established, and the energetics of thermally activated wall motion will be addressed.

399. **THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES**
J. V. Maher, Department of Physics and Astronomy
(412) 624-9007 02-2 $114,000

It is proposed to study 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-late anisotropy on patterns in a Hele-Shaw cell under a variety of conditions, in all cases with 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.

400. **DESIGNING INTERFACIALLY ACTIVE COPOLYMERS THROUGH MODELING AND STIMULATION**
A. C. Balazs, Department of Materials Science and Engineering
(412) 648-9250 03-2 $50,833

Computer simulations and theoretical models to examine how the self-association reactions of amphophilic 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 structure for such applications as stearic stabilization, adhesion and film growth. The approach involves using statistical mechanics, molecular dynamics and Monte Carlo computer simulations to model the polymer-surface interactions. These studies can allow the determination of how varying molecular structure or the chemical environment affects the properties of the interface.

## POLYTECHNIC UNIVERSITY

**Six MetroTech Center**
**Brooklyn, NY 11201**

401. **PROCESSING, DEFORMATION AND MICROSTRUCTURE OF SINGLE CRYSTAL $L1_0$ TYPE INTERMETALLIC COMPOUNDS**
S. H. Whang, Department of Metallurgy and Materials Science
(718) 260-3144 01-2 $150,000 (18 months)

Processing, deformation, and microstructural characterization of single crystals $L1_0$ type TiAl and CoPt compounds to elucidate mechanical property-microstructure relationship, in particular in relationship with the anomalous hardening in TiAl. Elastic constants and TEM observations of dislocation structures will be employed to develop theoretical models to explain the deformation mechanism and fracture behavior in TiAl.

402. **SCANNING TUNNELING MICROSPECTROSCOPY OF SOLIDS AND SURFACES**
E. L. Wolf, Department of Physics
(718) 260-3080 02-2 $95,999

Development of Scanning Tunneling Microscopy (STM) techniques for the study of solids and their surfaces. Investigation of the normal and superconducting states of high-$T_c$ materials, such as $Bi_2Sr_2CaCu_2O_8$, to obtain information about pair symmetries, density of states, gap energies, flux lattices, tunneling phenomena, and proximity effects as functions of temperature, oxygen stoichiometry, intercalation doping species, and external magnetic fields. Study of electron states and transport in mesoscopic metals and nanoscale structures.

403. **SHORT RANGE ORDER EFFECTS: CERIUM AND ACTINIDE MATERIALS**
P. Riseborough, Department of Physics
(718) 260-3675 02-3 $56,029

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 an 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

**Princeton, NJ 08544**

404. **VISCOELASTICITY OF POLYMER MELTS**
W. W. Graessley, Department of Chemical Engineering
(609) 258-5721 01-2 $92,400 (14 months)

Influence of molecular weight distribution in linear polymers and effects of long-chain branching on viscoelastic properties. A variety of model materials will be used in experimental portion, including unsymmetrical star polymers as well as linear chains and symmetrical stars in the form of binary mixtures. Develop a theoretical framework for polymer melt dynamics that includes a wide-variety of chain architectures.

405. **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.

406. **CONSOLIDATION OF COLLOIDAL DISPERSIONS; FILTRATION/SEDIMENTATION, FLOCCULATION AND PHASE SEPARATION**
W. B. Russel, Department of Chemical Engineering
(609) 258-4590 01-3 $60,000 from prior year

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.

407. **SURFACE STRUCTURE AND STEREOCHEMICAL PROPERTIES OF SELF-ASSEMBLED MONOLAYER MATERIALS**
G. Scoles, Department of Chemistry
(609) 258-5570 03-2 $59,652 (6 months)

Fundamental investigation of the self-assembly at metallic surfaces of substituted long-chain hydrocarbons with complex head groups. Use of both low energy atom diffraction and grazing incidence X-ray diffraction for structural characterization of monolayers of the chain hydrocarbons as a function of the chemical composition of their respective terminal groups. Determination of relative positions, alignment and orientations of the terminal groups not only as a function of the chain length of the supporting hydrocarbon but also as a function of temperature. Measurement of the stereoreactivity of the functional groups, such as double bonds and halogen substituted methyl groups, by exposure of the monolayers to collimated fluxes of reactive species (e.g., oxygen and fluorine; and the determination of the reaction probabilities as a function of direction and energy of the incoming species. Specific examples of monolayer systems used in the studies are $C_6H_{13}SH$ and $C_{22}$ chains and with either $-CH_2Br$ or $-CH=CH_2$ terminal groups.

## PURDUE UNIVERSITY
**West Lafayette, IN 47907**

408. **BEAMLINE 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 beamline at NSLS for all MATRIX members, and to support part of the research on phase transformation studies, X-ray surface and interface studies.

409. **STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA**
H. Sato, School of Materials Engineering
(317) 494-4099 01-3 $82,430

Research on multicomponent diffusion under general thermodynamical potential gradients. Chemical diffusion processes in alloys, different paths in ternary alloys with ordered regions, effects of ordering. Interdiffusion at boundaries, microscopic mechanisms of atomic exchange across boundaries. Interdiffusion in artificial superlattices in semiconductors.

410. **MIDWEST SUPERCONDUCTIVITY CONSORTIUM**
A. L. Bement, Department of Materials Engineering and Physics
(317) 494-5567 01-5 $2,700,000

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.

411. **GAMMA SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION**
J. R. Mullen, Department of Physics
(317) 494-3031 02-2 $130,000

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 constructed 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.

412. **ELECTRONIC AND STRUCTURAL PROPERTIES OF INDIVIDUAL NANOMETER-SIZE SUPPORTED METALLIC CLUSTERS**
R. G. Reifenberger, Department of Physics
(317) 494-3032    02-2 $62,000 from prior year

Investigation of the photo-excitation process at low photon energies. Techniques under development directly measure the excited state energy distribution of electrons that are emitted through the surface potential barrier. The fundamental process; photo-excitation of electrons from field emission tips by a focussed argon-ion laser beam tuned to operate at a specific photon energy. 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**

413. **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
**317A East Hall**
**Kingston, RI 02881-0817**

414. **SURFACE PHYSICS WITH COLD AND THERMAL NEUTRON REFLECTOMETRY**
A. Steyerl, Department of Physics
(401) 792-2204    02-1 $70,026

It is proposed to extend the methods of surface reflectometry to the use of ultra cold neutrons. This offers the unique possibility to improve the experimental sensitivity to the point where extremely small momentum and energy transfers relevant in critical surface phenomena will be accessible to experiment. A combination of the ultracold neutron technique 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 77251-1892**

415. **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

Exploitation of spin-sensitive surface spectroscopies 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), Spin-Polarized Metastable Deexcitation Spectroscopy (SPMDS), and other evolving spin-polarized spectroscopic techniques provide the experimental tools. Development of a spin-polarized $He^+$ ion beam and a superthermal $He(2_3S)$ metastable atom sources.

## UNIVERSITY OF ROCHESTER
**Rochester, NY 14627**

416. **MICROSTRUCTURAL BEHAVIOR OF NON-EQUILIBRIUM SYSTEMS**
J. C. M. Li, Department of Mechanical Engineering
(716) 275-4038    01-2 $90,049 from prior year

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.

417. **DYNAMICS OF SURFACE MELTING**
H. E. Elsayed-Ali, Laboratory for Laser Energetics
(716) 275-5101 03-3 $0 (0 months)

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**

418. **MECHANISMS OF MECHANICAL FATIGUE IN CERAMICS**
B. N. Cox, Science Center
(805) 373-4128

D. B. Marshall, Science Center
(805) 373-4170

W. L. Morris, Science Center
(805) 373-4545 01-2 $102,893

Investigate the relationship between microstructure and fatigue behavior in fiber/whisker and metal reinforced ceramics. Distinguish crack bridging and crack-tip-shielding mechanisms by very precise measurements of crack opening displacements and 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.

## STATE UNIVERSITY OF NEW JERSEY RUTGERS
**Piscataway, NJ 08855**

419. **THERMODYNAMIC AND KINETIC BEHAVIOR OF SYSTEMS WITH INTERMETALLIC AND INTERMEDIATE PHASES**
A. G. Khachaturyan, Department of Mechanics and Materials Science
(908) 932-2888

T. Tsakalakos and S. Semenovskaya, Department of Mechanics and Materials Science
(908) 932-4711 01-1 $155,040

Development of theoretical and computational simulation methods which can study the diffusional (ordering and decomposition) and martensitic transformations in metal alloys and complex ceramics over different temperature and stoichiometry ranges.

420. **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.

## SOUTH CAROLINA STATE UNIVERSITY
**Orangeburg, SC 29117**

421. **CHARACTERIZATION AND THERMOPHYSICAL PROPERTIES OF BI-BASED CERAMIC SUPERCONDUCTORS: PART A**
J.E. Payne, Department of Physics
(803) 536-7111 01-3 $165,460

The measurement of the heat capacity of YBCO and BISCCO single crystal superconductors are performed. Because available single crystals are small, microcalorimetry techniques, suitable for measuring submilligram insight into the origin of the superconductivity state, and characterizing the electron-phonon-interaction.

## UNIVERSITY OF SOUTHERN CALIFORNIA
**Los Angeles, CA 90089**

422. **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 polycrystalling (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.

423. **SYNTHESIS AND CHARACTERIZATION OF SELF-ASSEMBLING WATER-SOLUBLE POLYMERS**
T. E. Hogen-Esch, Department of Chemistry
(213) 740-5980

E. J. Emis, Department of Chemistry
(213) 743-6913 03-1 $95,000

Synthesis of water-soluble vinyl and other polymers capable of self-assembly through hydrophobic bonding of pendent fluorocarbon and other hydrophobic groups. Study of the self-assembly process by viscometry and dynamic viscoeleasticity, and by static and dynamic light scattering. Identification of polymer structural features that are important in enhancing the viscosity of aqueous polymer solutions at polymer concentrations below 1000 ppm. Small angle neutron scattering measurements to determine the size of the fluorocarbon containing hydrophobic aggregates. Investigation of the degree of self assembly as a function of the type and length of the hydrophobic groups and the type and length of flexible spacer groups linking the hydrophobic to the polymer backbone. Study of some hydrophilic comonomers such as acrylamide, N-vinylpyrrolidone and anionic or cationic vinyl monomers. Surface interactions studied by adsorption of copolymers onto appropriately modified latex spheres. Exploration of they synthesis of water-soluble polymers capable of self assembly through interactions of pendent polyanions and polycations.

## SOUTHWEST RESEARCH INSTITUTE
**6220 Culebra Road**
**San Antonio, TX 78238**

424. **CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING DENSIFICATION**
R. A. Page, Department of Materials and Mechanics
(210) 522-3252

K. S. Chan, Department of Materials and Mechanics
(210) 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**

425. **FUNDAMENTAL STUDIES ON PASSIVITY AND PASSIVITY BREAKDOWN**
D. D. Macdonald, Chemistry and Chemical Engineering Laboratories
(415) 859-3195

M. Wrquidi-Macdonald, Chemistry and Chemical Engineering Laboratories
(415) 859-3195 01-3 $191,394

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**

426. **MECHANICAL PROPERTIES OF MATERIALS WITH NANOMETER SCALE MICRO-STRUCTURES**
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 wavelengths 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.

427. **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 from prior year

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.

428. **ULTRA-LOW TEMPERATURE PROPERTIES OF AMORPHOUS AND CRYSTALLINE SOLIDS**
D. D. Osheroff, Department of Physics
(415) 723-4228 02-2 $112,000

The low temperature dielectric properties of amorphous systems are being investigated. The correlation between properties and the density of two level systems is being examined to understand low temperature saturation effects and to test for the importance of interactions. Thin film glass thermometry is being developed and applied to the study of heat capacities of crystalline materials at ultra-low temperatures to elucidate the nature of disorder in crystalline systems.

429. **A QUEST FOR A NEW SUPERCONDUCTING STATE**
J. P. Collman, Department of Chemistry
(415) 725-0283

W. A. Little, Department of Physic
(415) 725-4233 03-1 $160,000

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

## STATE UNIVERSITY OF NEW YORK AT BUFFALO
**Buffalo, NY 14214**

430. **SUNY BEAMLINE FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE**
P. Coppens, Department of Chemistry
(716) 831-3014 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.

431. **X-RAY STUDIES OF MICROSTRUCTURES IN SEMICONDUCTORS AND SUPERCONDUCTING MATERIALS**
Y. H. Kao, Department of Physics and Astronomy
(716) 636-2576 02-2 $100,000

Investigation of the short-range-order microstructure in layered materials and a new class of III-V diluted magnetic semiconductors. Experimental methods will include 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 will be prepared and characterized by collaborators at IBM.

## STATE UNIVERSITY OF NEW YORK AT STONY BROOK

**Stony Brook, NY 11794**

432. **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 on metals, and ordered surface alloys. Auger-electron spectroscopy will be 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), both in the angle-integrated and in the angle-resolved mode, is to be utilized.

433. **DESIGN OF SUPRAMOLECULAR ORDERED SYSTEMS FOR MESOSCOPIC COLLOIDS AND MOLECULAR COMPOSITES**

B. Chu, Department of Chemistry
(516) 632-7928 03-2 $58,250 (6 months)

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 rod-like polymers and functionlized rod (hairy rod) polymers. Synthesis and characterization of molecular composites based supermolecular structures.

434. **DETERMINATION OF CONCENTRATION PROFILES AT INTERFACES AND SURFACES OF PARTIALLY MISCIBLE POLYMER BLENDS**

M. Rafailovich, Department of Materials Science and Engineering
(516) 632-8483

J. Sokolov, Department of Materials Science and Engineering
(516) 632-8483 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 deutereated 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 make possible for the first time unique solutions to the concentration profiles, which will form the experimental basis for critical discrimination between current molecular theories.

## UNIVERSITY OF TENNESSEE

**Knoxville, TN 37996-0140**

435. **INVESTIGATIONS OF THE EFFECTS OF ISOTOPIC SUBSTITUTION AND PRESSURE ON MISCIBILITY IN POLYMER-POLYMER AND POLYMER-SOLVENT SYSTEMS**

A. Van Hook, Department of Chemistry
(615) 975-5105 03-2 $125,000

Measurement of phase separation temperature and related properties as a function of isotopic labeling (H/D) and pressure in polymer-polymer and polymer-solvent systems. Comparison, through the use of statistical theory of isotope effects in condensed phases, of isotope effect and pressure effects on the thermodynamic properties of solution, in particular the consulate properties. These measurements will be used to refine present molecular models of polymer-polymer and polymer-solvent interactions.

The results will aid in the interpretation of neutron scattering data in H/D mixtures of polymers.

## UNIVERSITY OF UTAH

**309 Park Building**
**Salt Lake City, UT 84112**

**436. 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 from prior year

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.

**437. THEORETICAL AND EXPERIMENTAL STUDY OF 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 GaInP, GaAsP, GaAsSb, GaInAsSb, GaPSb, InPSb, and InAsSb.

**438. FABRICATION, PHASE TRANSFORMATION STUDIES AND CHARACTERIZATION OF SIC-ALN-$AL_2OC$ CERAMICS**

A. V. Virkar, Department of Materials Science and Engineering
(801) 581-5396 01-1 $103,238

Phase equilibria, diffusional phase transformations and morphology of resultant phases and structure-property relations in the SiC-AlN-$Al_2OC$ system, with emphasis on SiC-AlN and AlN-$Al_2OC$ pseudobinaries. Interdiffusion measurements by Boltzmann-Matano method for AlN-$Al_2OC$ and SiC-AlN; kinetics of late stages and phase transformation in the AlN-$Al_2OC$ system; kinetics of early stage coherent spinodal phase separation in the AlN-$Al_2OC$ and SiC-AlN systems; effect of strain energy on phase separation; computer simulation of morphology of phase separation; potential for nanocomposite formation in the SiC-AlN and AlN-$Al_2OC$ systems. Samples fabricated by hot-pressing; characterization by TEM and XRD.

**439. ALUMINA REINFORCED TETRAGONAL ZIRCONIA POLYCRYSTAL (TZP) COMPOSITES**

D. K. Shetty, Department of Materials Science and Engineering
(801) 581-6449 01-2 $79,827

Transformation toughening and reinforcement in composites; alumina particle, platelet/whisker or fiber reinforcement of ceria- or yttria-partially stabilized zirconia (Ce-TZP or Y-TZP). Establishment of fiber stress-crack opening relation for crack-bridging in SiC (filament)-glass composites by laser raman spectroscopy. Matrix cracking in SiC-glass and $Al_2O_3$-Y-TZP composites in uniaxial tension. Processing of Y-TZP/$Al_2O_3$ platelet composites to improve fracture toughness and strength. Synergistic effects of fiber and transformation toughening in Y-TZP/$Al_2O_3$ filament (Saphikon) composites.

**440. THE SYNTHESIS OF MOLECULE/POLYMER-BASED MAGNETIC MATERIALS**

J. S. Miller, Department of Chemistry
(801) 581-6681 03-1 $60,334 (6 months)

The systematic synthesis and chemical characterizations of: glass-like $V(TCNE)_x$.y (solvent) as a function of solvent and replacement of the TCNE with other acceptors using new growth methods, including the growth of single crystals; metal cyclopentadienyl-TCNE complex solid solutions to investigate spin-spin coupling; new magnetic materials based upon metal cyclopentadienyl complexes with various, new acceptor molecules; and new systems exhibiting magnetic ordering, such as monolayers of $(RNH_3)_2CrCl_4$, where R is a long alkyl group capable of self-assembly. Continued collaboration with A. J. Epstein at the Ohio State University.

441. **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 from prior year

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.

442. **TRANSIENT AND CW OPTICAL STUDIES OF CONDUCTING POLYMERS**
Z. V. Vardeny, Department of Physics
(801) 581-8372 03-2 $112,000

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**

443. **CLUSTERS AND CLUSTER REACTIONS**
P. Jena and S. N. Khanna, Physics Department
(804) 367-1313

B. K. Rao, Physics Department
(804) 257-1313 01-3 $151,934

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**

444. **CHARACTERIZATION OF SUPERCONDUCTING MATERIALS WITH MUON SPIN ROTATION**
C. E. Stronach, Department of Physics
(804) 524-5915 01-3 $149,135

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
**Thornton Hall**
**Charlottesville, VA 22903**

445. **HETEROGENEOUS NUCLEATION IN METAL ALLOYS**
G. J. Shiflet, Department of Materials Science and Engineering
(804) 982-5653 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, 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.

446. **SURFACE STRUCTURE AND ANALYSIS WITH SCANNING TUNNELING MICROSCOPY AND ELECTRON TUNNELING SPECTROSCOPY**
R. V. Coleman, Department of Physics
(804) 924-3781 02-2 $75,000 (7 months)

Development of scanning tunneling microscopy (STM) and atomic force microscopy (AFM) techniques with emphasis toward improving the observation of surface atomic configurations and the measurement of associated electronic states. Particular attention given to techniques which can be applied over a range of temperature, vacuum conditions and applied magnetic fields. Application of STM and AFM to investigation of the intercalation of transition metal impurities into dichalcogenides and the spatial and magnetic superlattices which result with intercalation. Studies of the detection, creation and manipulation of defects in layered chalcogenides. Investigation of the oxidation processes on iron surfaces and the etch pits at radiation damage tracks in mica.

447. **SUPERCONDUCTING MATERIALS**
J. Ruvalds, Department of Physics
(804) 924-3781 02-3 $77,000 (11 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 will be on quasiparticle damping in view of the anomalous 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 anomalous susceptibility.

## WASHINGTON STATE UNIVERSITY
**Pullman, WA 99164**

448. **A STUDY OF TRANSIENT PARTICLE COARSENING**
J. Hoyt, Department of Mechanical and Materials Engineering
(509) 335-8523 01-1 $58,129 (14 months)

Study of the transient particle coarsening in Al-Li alloys. TEM used to measure average particle size and size distribution. SAXS used to determine ratio of second to third moments of particle size distribution function. Measured time dependence to be compared to numerous coarsening theories.

449. **METAL INDUCED EMBRITTLEMENT**
R. G. Hoagland, Department of Mechanical and Metallurgical Engineering
(509) 335-8280 01-2 $54,436

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 63130-4899**

450. **MULTI-BODY FORCES AND ENERGETICS OF TRANSITION METALS, ALLOYS, AND SEMICONDUCTORS**
A. E. Carlsson, Department of Physics
(314) 935-5739 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**

451. **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 spectroscopy. Emphasis is on the study of materials undergoing pressure induced phase transitions such as the bcc to hcp transformation in metallic iron and structure 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.

452. **NEAR-EDGE X-RAY SPECTROSCOPY THEORY**
J. J. Rehr, Department of Physics
(206) 543-8593 02-2 $43,641 (14 months)

A theoretical-calculational investigation of various deep core X-ray spectroscopies such as X-ray absorption fine structure (XAFS), photoelectron diffraction (PD), and diffraction anomalous fine structure (DAFS). Development, maintenance, and distribution of computer codes to provide a state-of-the-art means to obtain a theoretical mimicry which can be compared with experimental XAFS-type spectra. Important features of the codes are portability and their ease of application to various

X-ray spectroscopies. All relevant multiple-scattering and atomic vibrations effects are included in the codes. Special emphasis placed on the theoretical development of improved treatment of many-body and electron self-energy effects with their eventual inclusion into the library of codes, which is important in order to obtain the best possible agreement between calculated and experimental spectra in their near-edge region (less than 100 eV).

453. **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.

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## UNIVERSITY OF WISCONSIN AT MADISON
**1509 University Avenue**
**Madison, WI 53706**

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454. **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 $92,082

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.

455. **GRAIN-BOUNDARY STUDIES IN IONIC CONDUCTORS**
E. E. Hellstrom, Department of Materials Sciences and Engineering
(608) 263-9462 01-3 $87,609 (14 months)

Investigation of the relationships between ionic conductivity across grain boundaries and the lattice misorientation, structural relaxation, segregation, and space charge at grain boundaries. Model system based on bicrystals and polycrystalline samples of lightly doped $CeO_2$. Characterization by AC and DC conductivity techniques, high-spatial-resolution analytical electron microscopy, Auger electron spectroscopy. Modelling of grain boundary segregation and space-charge layer.

456. **ELEMENTAL AND MULTILAYER LARGE MOMENT THIN FILM FERROMAGNETS**
M. Onellion, Department of Physics
(608) 263-6829 02-2 $60,000

Fabrication of magnetic films and heterostructures by metal-organic chemical vapor deposition (MOCVD) and other techniques. Application of the Magneto-Optic Kerr Effect (MOKE) and electron photoemission to the characterization of magnetic films, bilayers, and trilayers of rare-earth and transition metals, and oxide/metal heterostructures. Examination of magnetic exchange within and between layers in heterostructures. Determination of magnitude and orientation of magnetic moments in rare- earth thin films and superlattices.

457. **MORPHOLOGICAL ANALYSIS OF IONOMERS**
S. L. Cooper, Department of Chemical Engineering
(608) 262-4502 03-2 $92,500

Synthesis of ionomers with regular placement of ionic groups along the chain. Small angle X-ray scattering techniques used to probe shape, size, and arrangements of ionic aggregates in ionomers. Effect of casting solvent, compression molding and solution casting on morphology. Determination of aggregate dissociation temperature. Anomalous small angle X-ray scattering (ASAXS) to resolve source of zero-angle upturn in scattering intensity. Tensile properties to monitor the dramatic cation influence, the effect of water, trends within a chemical group and the effect of anion type. SANS experiments using deuterated polyols will measure temperature dependence, response to deformation and be interpreted for cation effects.

## UNIVERSITY OF WISCONSIN AT MILWAUKEE
**Milwaukee, WI 53201**

458. **UNDULATOR SPECTRO-MICROSCOPY FACILITY AT THE ADVANCED LIGHT SOURCE**
B. P. Tonner, Department of Physics
(414) 229-4626 02-2 $100,000

This grant supports part of a proposal to design and construct a beamline at the Advanced Light Source. The grant will pay for 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. This is 5 times greater than the current state-of-the-art instrument. The spectral resolution of the instrument will be a maximum of 0.1 eV. Specifications for the holography and photoelectron diffraction systems will be drawn up, and sent out for bid. Complete ray tracing for the beamline will be performed to determine the optimal configuration for the SPEM optics.

459. **INELASTIC ELECTRON SCATTERING FROM SURFACES**
S. Y. Tong, Department of Physics
(414) 229-5765 02-3 $96,000 from prior year

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.

## WORCESTER FOUNDATION FOR EXPERIMENTAL BIOLOGY
**Shrewsbury, MA 01545**

460. **NOVEL BIOMATERIALS: GENETICALLY ENGINEERED PORES**
H. Bayley
(508) 842-9146 03-2 $83,000 (6 months)

A section of nanometer-scale pores is being constructed by genetic manipulation of α-hemolysin (αHL), a protein secreted by the bacterium Staphylococcus aureus. The single polypeptide chain of 293 amino acids forms hexameric pores in membranes ~11A in internal diameter. Our recent focus has been on the mechanism by which the pore assembles. By analyzing the properties of truncation mutants and two-chain complementation mutants and by studying the chemical modification of single-cysteine mutants, a working model for assembly has been devised. Monomeric αHL binds to lipid bilayers and undergoes a conformational change (involving the occlusion of a central glycine-rich loop) that allows the formation of a hexameric prepore complex. The open more is formed when subunits in this complex undergo a second conformational change after which they span the bilayer. Our studies identified the regions of αHL that are important in each step in assembly and thereby have permitted the design of αHL polypeptides in which pore-forming activity is modulated by biochemical, chemical or physical triggers and switches. For example, αHL polypeptides with modified central loops can be activated by specific proteases or reversibly inactivated by divalent cations. Now, point mutagenesis and chemical modification are being used to create pores with different internal diameters, with selectivity for the passage of molecules and ions, and which are gated by a variety of inputs. Ultimately, the new pores will be used to confer novel permeability properties upon materials such as thin films, which might be used as components of energy conversion and storage devices, selective electrodes, electronic devices, and ultrafilters. * Funded collaboratively with Energy Biosciences.

**YALE UNIVERSITY**
**New Haven, CT 06520**

461. **MICROSTRUCTURAL DEPENDENCE OF THE CAVITATION DAMAGE POLYCRYSTALLINE MATERIALS**
B. L. Adams, Department of Mechanical Engineering
(203) 432-0159 01-2 $0 (0 months)

Establish microstructural and stress state dependence of cavitation damage in F.C.C. metal alloys. Experimental and analytical studies to define a Cavitation-Damage Function under multi-axial loading. Technique involves measuring local crystallite orientations adjacent to grain boundaries of sectioned samples using Electron Backscattering Diffraction. Materials are Type 304 stainless steel and copper alloys.

# SECTION C

Small Business Innovation Research

## ADVANCED FUEL RESEARCH, INC.

**87 Church Street**
**East Hartford, CT 06138-0379**

462. **IN-SITU PARTICLE SENSOR FOR METAL FORMING PROCESSES**
S. Farquharson
(203) 528-9806 Phase II SBIR $74,957

Numerous processes are being developed for the manufacturing of advanced composites which incorporate ceramics, polymers, metals and/or metal alloys. The success of these manufacturing processes is critically dependent on the ability to both monitor and control the processing conditions. Of particular interest is the development of powdered metals as a source materials for a variety of metal forming processes, such as plasma spray, sintering, and hot isostatic pressing. However, a lack of sensors is slowing the development of the powder technology. This project will develop and field test a metal powder smart-sensor which can be employed in the hot particle forming plume, in the following stream of formed particles, and as part of a sizing system to characterize collected particles. The technique employs Fourier Transform.

463. **IN-SITU PARTICLE SENSOR FOR METAL FORMING PROCESSES**
S. Farquharson
(203) 528-9806 Phase II SBIR $74,957

Numerous processes are being developed for the manufacturing of advanced composites which incorporate ceramics, polymers, metals and/or metal alloys. The success of these manufacturing processes is critically dependent on the ability to both monitor and control the processing conditions. Of particular interest is the development of powdered metals as a source material for a variety of metal forming processes, such as plasma spray, sintering, and hot isostatic pressing. However, a lack of sensors is slowing the development of the powder technology. This project will develop and field test a metal powder smart-sensor which can be employed in the hot particle forming plume, in the following stream of formed particles, and as part of a sizing system to characterize collected particles. The technique employs Fourier Transform Infrared (FT-IR) spectroscopy to differentiate the scattering of various particle sizes. FT-IR Scattering (FT-IRS) spectroscopy relies on the wavelength dependence of light scattering rather than the angular dependence employed by other techniques. In addition, FT-IR emission spectroscopy in combination with FT-IRS offers a unique capability for particle temperature measurements in the plume. Because of the FT-IR's capabilities, a single spectrometer will be able to monitor particle size distributions and temperatures in a process stream, and issue process control commands. In Phase I an FT-IR instrument for in situ particle analysis of the plume of a metal powder facility (MPF) will be developed and field tested. The instrument development would include coupling of two detectors for long and short wavelength measurements, the development of optics to couple the instrument to the MPF, the development of a calibration system, and fast data acquisition and analysis algorithms applicable to high-rate metal forming processes. Field testing will occur over a one to two week period in the fifth month of the program.

## ADVANCED OPTICAL TECHNOLOGIES, INC.

**628 Hebron Avenue**
**Glastonbury, CT 06033**

464. **A HIGH COUNT RATE TWO-DIMENSIONAL NEUTRON DETECTOR**
Y.-S. Chao
(203) 657-2668 Phase II SBIR $74,639

Most major neutron facilities operating in the U.S. were developed two or three decades ago. To meet the new challenges for materials and biological research in the future, a new generation of neutron facilities with must higher flux and with compatible instrumentation is being considered. The current technology of neutron detection (gas-filled, proportional, position-sensitive chambers) could not meet the needs in an advanced neutron source environment because of the inherently limited maximum count rate, limited spatial resolution, and limited detection efficiency, especially for neutrons with shorter wavelength. To meet the needs for neutron scattering and neutron diffraction experiments at higher neutron fluxes, this Phase I project will study the development of a large format, integrated, amorphous silicon, photodiode array coupled with an efficient scintillator. The novel two-dimensional neutron detector is expected to be able to improve the maximum count rate from the current $10_5$-$10_6$/second given by a gas-filled chamber to $10_8$-$10_9$/second, resulting in significantly improved productivity and data throughput. Spatial resolution is expected to be enhanced from the current 5 mm level to a submillimeter level. Parallax error produced by gas-filled detectors will be eliminated, and at the same time detection efficiency for shorter wavelength (down to 0.5A) neutrons would also be substantially improved. Phase I should demonstrate feasibility of the planned approach, and Phase II would provide a prototype two-dimensional neutron detector.

## ADVANCED RESEARCH AND APPLICATIONS CORPORATION

**425 Lakeside**
**Sunnyvale, CA 94086**

### 465. A WAVELENGTH DISPERSIVE SPECTROMETER FOR ANALYTICAL ELECTRON MICROSCOPY

E. D. Franco
(408) 733-7780 Phase II SBIR $75,000

The development of a novel non-scanning wavelength dispersive spectrometer (WDS) for analytical electron microscopy (AEM) is the objective of this project. This spectrometer is designed to provide sufficient energy resolution over broad regions of the soft X-ray spectral region (from 100 to 2000 eV) to allow the observation of the K-emissions of the light elements (those with atomic numbers less than 10) as well as the L, M, and N emissions of the heavy elements. The large solid angle of this spectrometer and its non-scanning geometry decrease the analysis time compared to conventional WDS instruments while offering at least a fourfold increase in spectral resolving power compared to energy dispersive detectors currently offered in the AEM marketplace. The Phase I objective is to experimentally evaluate the performance of a prototype spectrometer in terms of lower limits of detection in the energy range from 150 to 300 eV in a re-entrant AEM environment. This objective will be accomplished by the fabrication of a single channel prototype of the spectrometer and the measurement of the signal and background levels in a modern AEM.

## BIOTRACES, INC.

**7986 Lakecrest Drive**
**Greenbelt, MD 20770**

### 466. DEVELOPMENT OF A HIGH SPATIAL RESOLUTION NEUTRON DETECTOR

A. K. Drukier
(301) 345-3279 Phase II SBIR $75,000

Neutron scattering studies have been usually carried out using single detectors. In the last few years, the use of spatially resolving detectors has resulted in better statistical accuracy with substantially reduced data collections times. Although, the commonly used neutron detector array consisting of multiwire He-3 camera is capable of excellent photonic background rejection, its use is severely limited due to low spatial resolution and count rate limitations. To overcome these difficulties, development of a new class of high spatial resolution neutron detectors based upon superconducting energy-sensitive structures is planned. A detector with a few square centimeter area, excellent spatial resolution, and high detection efficiency will be developed. The crucial component of this detector will be a large array (2048 x 2048) of superconducting sensors deposited on the surface of a neutron absorber (e.g., boron, boron nitride, or lithium hydride) which will act as a neutron to alpha particle "converter." Such a detector can attain a spatial resolution of a few tons of microns with a reasonable number (<256) of readout channels. In Phase I, a prototype detector on the surface of a boron nitrite substrate will be fabricated. Furthermore, a multichannel electronic readout system will be developed to enable quantitative measurements of the spatial resolution and quantum detection efficiency.

## INRAD, INC.

**181 Legrand Avenue**
**Northvale, NJ 07647**

### 467. SINGLE CRYSTAL MOLYBDENUM MIRRORS FOR HIGH POWER X-RAY SYNCHROTRONS

W. Ruderman
(201) 767-1910 Phase II 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 producing 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. The Phase II program 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 energies from 100 eV to 10 keV for representative samples will be made at the National Synchrotron Light Source at the Brookhaven National Laboratory.

## MULTILAYER OPTICS AND X-RAY TECHNOLOGY, INC.

**7070 University Station**
**Provo, UT 84602**

468. **WAVELENGTH DISPERSIVE X-RAY SPECTROMETERS FOR ANALYTICAL 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.

## NANOPTICS, INC.

**3014 NE 21st Way**
**Gainesville, FL 32609**

469. **HIGH RESOLUTION SCINTILLATOR-BASED NEUTRON DETECTOR**
W. Y. Choi
(904) 378-6620 Phase II SBIR $75,000

A novel technology for a scintillator-based neutron converter plate which will have high thermal neutron detection efficiency (~90%) and inherently high spatial resolution is planned. The neutron converter plate will be made using scintillating plastic micro-fibers with enriched lithium ($_6$Li) incorporation. This neutron converter overcomes the fundamental problems associated with screen phosphors and will be a superior alternative. The detector can be used either for a time-integating imaging mode or for a conventional time-resolved position sensitive detector mode. Phase I will develop and test the novel neutron converter plate. Measurements will include neutron detection efficiency, scintillation efficiency, absorption/emission spectrum, and decay time of the scintillator. The results of Phase I will demonstrate the effectiveness of the converter plate compared with those obtained from standard screen phosphors. In Phase II, a complete real-time thermal neutron imaging system using the neutron converter will be built and applied to various thermal neutron imaging applications.

## PEAK INSTRUMENTS, INC.

**112 West Franklin Avenue**
**Pennington, NJ 08534**

470. **AN EFFICIENT X-RAY WAVELENGTH SPECTROMETER FOR IMPROVED ELEMENTAL ANALYSIS ON ELECTRON MICROSCOPES**
Barbi N. C.
(609) 737-8133 Phase II SBIR $399,601

A new type of wavelength dispersive (WD) X-ray spectrometer is planned. Its anticipated attributes include: (1) high efficiency with high resolution; (2) small physical size; and (3) high-vacuum compatibility. These improvements potentially enable wavelength spectroscopy to be performed on several types of electron microscopes (EMs) currently unsuitable for WD spectrometer: (1) analytical electron microscopes (AEMs), which require a great reduction in spectrometer size; (2) large-chamber scanning electron microscopes (SEMs), which require larger Rowland circles than presently available or likely to become available (due to reduce efficiency); (3) cold field-emission SEMs, which, due 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 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 convectional WD systems. Compared to energy dispersive spectrometers commonly used on all of the above instruments, the proposed spectrometer will provide more sensitive analysis, particularly for the light elements.

## X-RAY INSTRUMENTATION ASSOCIATES
**1300 Mill Street**
**Menlo Park, CA 94025-3210**

471. **DIGITAL PROCESSING ELECTRONICS FOR X-RAY DETECTOR ARRAYS**
W. K. Warburton
(415) 903-9980 Phase II SBIR $50,000

Many areas of synchrotron radiation investigation are severely detector limited, particularly 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 presently restricted by the cost, physical size, and complexity of the required analog processing electronics. In Phase I, detailed studies were performed, investigating the possibility of developing digital processing electronics based on concepts of digital signal processing. By both hardware and software modeling studies, it was shown that it is possible to match the resolution of current analog systems while increasing maximum throughput by a factor of 2, decreasing costs by factors of 4 to 8, and reducing physical size by an order of magnitude. If these gains can be demonstrated in practice, then arrays with 100 or more channels will become practical. Phase II will address the issues involved in physically realizing a digitally based signal processing system. The work is particularly directed toward resolving issues of signal preconditioning, constructing a hardware filter and control system, and demonstrating a route to cost effective commercialization. A successful project will result in a working demonstration unit.

## X-RAY OPTICAL SYSTEMS
**1400 Washington Avenue**
**Albany, NY 12222**

472. **A COLD/THERMAL BEAM BENDER USING CAPILLARY OPTICS TO INCREASE THE NUMBER OF END-GUIDE INSTRUMENT POSITIONS**
Q. Xiao
(518) 442-5250 Phase II SBIR $50,000

The use of promising non-destructive cold and thermal neutron material analysis techniques has been hindered by the limited availability of high-flux sources of low-energy neutrons. This project will develop neutrons benders which 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 guide. This neutron optics utilizes glass capillaries with small diameter channels through which the neutrons make multiple reflections at less than the critical angle of reflection. Phase I demonstrated high transmission efficiency through individual polycapillaries which were over 50 cm long an deflected the beam by more than 10°. Computer simulations and experimental results were in very good agreement for borosilicate glass. The design and construction of a neutron bender for Prompt Gamma Activation Analysis (PGAA) and Small Angle Neutron Scattering (SANS) was determined to be feasible. Phase II will develop and test full size prototypes customized for prompt gamma activation analysis and small-angle neutron scattering. The optics design will be tailored to meet the application requirements: providing filtration of gamma rays and epithermal neutrons, collimating the beam, and/or focusing the beam for good spatial resolution. Phase II will involve collaboration with experienced personnel from multiple reactor site.

# 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.l-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 (4 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>0.01 E |
| Glass, Liquid and Amorphous Materials Diffractometer (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.
Two sample positions
<-> Elastic and inelastic resolution

**Not Yet in the User Program**
***Small Angle Neutron Diffractometer (SAND, 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
Brookhaven National Laboratory — Fax (516) 282-5888
Building 510A
P. O. Box 5000
Upton, NY 11973-5000

# 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 wave-length 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 $< \lambda <$ 4.0 Å 2d detector with time slicing electronics and on-line data analysis. |
| 2 Diffractometers (H6S, H6M) | Single-crystal elastic scattering 4-circle goniometer 1.69 Å $< \lambda_o <$ 0.65 Å |
| 1 Triple-axis Spectrometer (H5) | Inelastic scattering<br>Diffuse scattering<br>Powder diffractometry |
| 2 Spectrometers (H1A, H1B) | Neutron capture studies<br>Energy range: 0.025 eV $< E_o <$ 25 KeV |
| TRISTAN II (Isotope Separator) (H2) | Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission |
| Irradiation Facilities | |
| 7 Vertical Thimbles | Neutron activation; production of isotopes; thermal flux: 8.3 x $10^{14}$ neutrons/$cm^2$-sec; fast (> 1.0 MeV) flux: 3 x $10^{14}$ neutrons/$cm^2$-sec. |
| Netron 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. $\lambda$ = 1.88Å, $\Delta d/d = 5 \times 10^{-4}$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 (VUV) ring which operates at an electron energy of 750 MeV designed for optimum radiation at energies between 10 eV and 1 keV, and an X-ray ring which operates at 2.5 GeV to optimize radiation between 1 keV and 20 keV. The X-ray ring accommodates 32 experimental ports and the VUV ring accommodates 20. Each of these ports can be split into two to four beam lines. By the end of 1993, the Light Source will have 83 operational experimental beamlines. Of these, four lines are dedicated to beam diagnostics.

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. Active General User programs are underway on most of the insertion device lines at the Light Source.

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, spin polarized photoemission). These are but a few of the exciting research opportunities at the NSLS. As of April 1, 1993, over 2572 scientists from 405 universities, laboratories, corporations and foreign institutions are registered users of the research tools available at the NSLS.

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. During FY 1993, eight corporations utilized 378 shifts of NSLS operations to conduct proprietary research.

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. Beamlines are either constructed by Participating Research Teams (PRTs), Insertion Device Teams (IDTs), or by Brookhaven staff members. The institutional representation on the PRTs and IDTs totals 83. Each PRT and IDT is entitled to up to 75% of their beam line's operational time for a three-year term. The remaining beam time is made available to scientists categorized as "General Users."

General users are scientists interested in using existing NSLS facilities for experimental programs. The NSLS runs three scheduling cycles per year. Access to the facility is through a proposal system. Proposals are reviewed by NSLS staff for technical feasibility, safety, and personnel resources, and checked by the cognizant beamline personnel for conformance to the beamline's capabilities. General User proposals are subject to review by a Proposal Study Panel. All beamline/time allocations are assigned by the NSLS General User Oversight Committee. Liaison and utilization support is provided to the General User by the cognizant beamline personnel. One hundred and seventy-three new General User proposals along with 256 beam time requests against existing proposals were submitted during FY 1992. A total of 2286 days of beam time were allocated to General Users on the X-ray and UV rings during FY 1992.

PERSON TO CONTACT FOR INFORMATION

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Upton, NY 11973

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bnl::ezr

## NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

### TECHNICAL DATA

| Storage Ring | Key Features |
|---|---|
| VUV electron | 17 ports; Ec - 25.3 angstroms; 0.745GeV electron energy |
| X-ray electron | 30 ports; Ec - 2.48 angstroms; 2.584GeV electron energy |

| Research Area | Wavelength Range (Å) | Energy Range (eV) | Number of Instruments |
|---|---|---|---|
| Absorption Spectroscopy | 0.35 - 2480 | 5 - 35,000 | 24 |
| Circular Dichroism | 10.3 - 5904 | 2.1 - 1200 | 2 |
| High Pressure Physics | 1 - 10,000μm<br>WB; 0.12 1.24 | 0.124 - 1240 meV<br>WB; 10,000 - 100,000 | 2<br>2 |
| High Q-Resolution Scattering | WB; 0.12 - 6.20 | WB; 2000 - 100,000 | 15 |
| Imaging | | | |
| - Medical | WB; 0.12 - 1.24 | WB; 10,000 - 100,000 | 2 |
| - Tomography | WB; 0.12 - 3.10 | WB; 4000 - 100,000 | 3 |
| - X-ray Microprobe | WB; 0.12 - 3.10 | WB; 4000 - 100,000 | 3 |
| - X-ray Microscopy/Holography | 10 - 80 | 155 - 1240 | 1 |
| - X-ray Topography | WB; 0.41 - 3.10 | WB; 4000 - 30,000 | 2 |
| Infrared Spectroscopy | 1 - 10,000μm | 0.124 - 1240 meV | 2 |
| Lithography | 124 - 4133 | 3 - 100 | 1 |
| Nuclear Physics | --- | 80 - 400 (meV) | 1 |
| Photoemission Spectroscopy | 2.10 - 6200 | 2 - 5900 | 19 |
| Photoionization | 2.10 - 4133 | 3 - 5900 | 3 |
| Protein Crystallography | WB; 0.41 - 3.10 | WB; 4000 - 30,000 | 6 |
| Radiometry | WB; 8.27 - 248 | WB; 50 - 1500 | 1 |
| Small Angle Scattering | | | |
| - Biology | 0.66 - 5.90 | 2100 - 18,800 | 2 |
| - Materials Science | 0.36 - 6.20 | 2000 - 34,000 | 4 |
| Small Molecule Crystallography | | | |
| - Powder | WB; 0.12 - 3.10 | WB; 4000 - 10,000 | 4 |
| - Single Crystal | 0.21 - 6.20 | 2000 - 59,400 | 7 |
| Standing Waves | WB; 0.31 - 6.89 | WB; 1800 - 40,000 | 3 |
| Surface Scattering/X-ray Reflectivity | WB; 0.48 - 6.20 | WB; 2000 - 26,000 | 10 |
| Time Resolved Fluorescence | 1393 - 5904 | 2.1 - 8.9 | 1 |
| UV Reflectometry | WB; 8.27 - 6200 | WB; 2 1500 | 2 |
| X-ray Emission Spectroscopy | 2.48 - 50 | 248 - 5000 | 2 |

WB = White Beam (from 1993 NSLS User's Manual - BNL 48724)

# 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 chopper spectrometer (PHAROS) for Brillouin scattering, 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.

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<br>diffractometer Wave vectors 1-15 $Å^{-1}$<br>Resolution 2% typical |
| Filter Difference Spectrometer<br>(J. Eckert, Responsible) | Inelastic neutron scattering,<br>vibrational spectroscopy<br>Energy trans. 15-600 meV<br>Resolution 5-7% |
| High Intensity Powder Diffractometer<br>(R. VonDreele, Responsible) | Powder diffraction .7% resolution;<br>liquids and amorphous materials<br>diffraction 2% resolution |
| Constant-Q Spectrometer<br>(R. Robinson, Responsible) | Elementary excitations in<br>single crystal samples<br>Energy resolution 1-3% |
| Low Q Diffractometer<br>(P. A. Seeger, Responsible) | Small angle scattering at a<br>liquid hydrogen cold source<br>Wave vectors 0.003-1.0 $Å^{-1}$ |
| Reflectometer<br>(G. Smith, Responsible) | Surface reflection at grazing<br>incidence. Wave vector range<br>0.007 to 0.3 $Å^{-1}$ |
| Chopper Spectrometer<br>(R. Robinson, responsible) | Inelastic scattering at small<br>scattering angles. Incident<br>energy resolution of 0.5%. |

# 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 six months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be born 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<br><br>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 LINEAR ACCELERATOR CENTER

**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 25 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. Environmental studies. Semiconductor and thin film processing. 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 6-7 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" provide detailed information on proposal submittal and experimental station characteristics.

PERSON TO CONTACT FOR INFORMATION

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

(415) 926-3191
Fax No.: (415) 926-4100

EMail: K@SSRL750 or K@SSRL01.SLAC.STANFORD.EDU

# CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

SSRL has 25 experimental stations on SPEAR. 13 of these stations are based on insertion devices while the remainder use bending magnet radiation.

| Station | Horizontal Angular Acceptance (Mrad) | Mirror Cut Off (keV) | Monochromator | Energy Range (eV) | Resolution E/E | Approximate Spot Size HgtxWdth (mm) | Dedicated Instrumentation |
|---|---|---|---|---|---|---|---|
| **INSERTION DEVICES STATIONS** | | | | | | | |
| Wiggler Lines - X-Ray | | | | | | | |
| End Stations | | | | | | | |
| 4-2 (4 periods) | | | | | | | |
| Focused | 4.6 | 10.2 | Double Crystal | 2800-10200 | $\sim 5\times10^{-4}$ | 1.0 x 3.0 | |
| Unfocused | 1.0 | | Double Crystal | 2800-45000 | $\sim 10^{-4}$ | 2.0 x 20.0 | |
| 6-2 (27 periods) | | | | | | | |
| Focused | 2.3 | 22 | Double Crystal | 2400-21000 | $\sim 5\times10^{-4}$ | 1.0 x 3.0 | |
| Unfocused | 1.0 | | Double Crystal | 2400-45000 | $\sim 5\times10^{-4}$ | 2.0 x 20.0 | |
| 7-2 (4 periods) | | | | | | | 6-circle Diffractometer |
| Focused | 4.6 | 10.2 | Double Crystal | 2800-10200 | $\sim 5\times10^{-4}$ | 1.0 x 3.0 | |
| Unfocused | 1.0 | | Double Crystal | 2800-45000 | $\sim 10^{-4}$ | 2.0 x 20.0 | |
| 10-2 (15 periods) | | | | | | | |
| Focused | 2.3 | 22 | Double Crystal | 2800-21000 | $\sim 5\times10^{-4}$ | 1.0 x 3.0 | |
| Unfocused | 1.0 | | Double Crystal | 2800-45000 | $\sim 10^{-4}$ | 2.0 x 20.0 | |
| Side Stations | | | | | | | |
| 4-1 | 1.0 | | Double Crystal | 2800-45000 | $\sim 5\times10^{-4}$ | 2.0 x 20.0 | |
| 4-3 | | | | | | | 2-circle Diffractometer |
| Focused | 1.0 | Variable | Double Crystal | 2800-20000 | $\sim 10^{-4}$ | 0.3 x 20 | |
| Unfocused | 1.0 | | Double Crystal | 2800-45000 | $\sim 10^{-4}$ | 2.0 x 20.0 | |
| 7-1 | 1.0 | | Curved Crystal | 6000-13000 | $\sim 8\times10^{-4}$ | 0.6 x 3.0 | Rotation Camera |
| 7-3 | 1.0 | | Double Crystal | 2800-45000 | $\sim 10^{-4}$ | 2.0 x 20.0 | |
| VUV/Soft X-ray Stations | | | | | | | |
| 5-1,5-3 multi-undulator | 1.5 | | 4 Gratings | 10-450 | $0.5\text{-}1\times10^{-3}$ | 2.0 x 3.0 | |
| 5-2 multi-undulator | 1.5 | | 4 Gratings | 10-1200 | $0.5\text{-}1\times10^{-3}$ | 2.0 x 3.0 | |
| 10-1 | 2.0 | | 6m SGM | 200-1000 | $\sim 2\times10^{-4}$ | $\leq$1mm$^2$ | |
| **BENDING MAGNET STATIONS** | | | | | | | |
| X-ray | | | | | | | |
| 1-4 | 2.0 | | Curved Crystal | 6700-10800 | $0.3\times10^{-3}$ | 0.25 x 1.0 | SAS Detector |
| 1-5 | 1.0 | | Double Crystal | 2800-30000 | $\sim 10^{-4}$ | 3 x 20 | Area Detector/CAD-4 |
| 2-1 (Focused) | 4.8 | 8.9 | Double Crystal | 2800-8900 | $\sim 5\times10^{-4}$ | 1 x 4 | |
| 2-2 | 1.0-6.1 | | None | 3200-40000 | | 4 x 22 - 4 x 134 | |
| 2-3 | 1.0 | | Double Crystal | 2800-30000 | $\sim 5\times10^{-4}$ | 3 x 20 | |
| VUV/Soft X-ray | | | | | | | |
| 1-1 | 2.0 | | Grasshopper | 64-1000 | =.1-.2A | 1.0 x 1.0 | |
| 1-2 | 4.0 | | 6m TGM | 8-90 | $\sim 1\times10^{-3}$ | 1.0 x 2.0 | |
| 3-1 | 2.0 | | Grasshopper | 25-1000 | =05.2A | 1.0 x 1.0 | |
| 3-2 | 4.0 | | Seya-Namioka | 5-40 | =.2-6A | 2 x 7 | |
| 3-3 | 8-10 | 4.5 | UHV Double Crystal (Jumbo) | 800-4500 | $\sim 5\times10^{-4}$ | 1.5 x 2.5 | |
| 3-4 | 0.6 | | Multilayer | 0-3000 | White or =.6% | 2 x 8 | Vacuum Diffractometer Litho.Expo. Station |
| 8-1 | 12 | | 6m TGM | 8-180 | $\sim 1\times10^{-3}$ | $\leq$1mm | |
| 8-2 | 5.0 | | 6m SGM | 150-1000 | $\sim 1\times10^{-4}$ | $\leq$1mm$^2$ | |

# 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, High-$T_c$ Update, 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 Lawrence L. Jones, Director, R. Tom Lograsso, MRSH Manager, 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 Lograsso, MRSH Manager, (515) 294-8900.

### High-$T_c$ Superconductivity Information Exchange

The newsletter, High-$T_c$ Update, is published twice-monthly and available without charge as either hard copy or electronic mail. Inquiries should be directed to Sreeparna Mitra, (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

Lawrence L. Jones, Director (515) 294-5236
Ames Laboratory
Materials Preparation Center
121 Metals Development Building
Ames, IA 50011

Thomas A. Lograsso (515) 294-8900
Ames Laboratory
Materials Preparation Center
109 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 μA/cm$^2$ (typical) $Ni^+$, 3 μA/cm$^2$ |
| NEC 650 kV Injector<br>Being acquired | Terminal voltage 650 kV<br>Energy stability ± 60 eV<br>Current density: $He^+$, 100 μA/cm$^2$ (typical) $Ar^+$, 10 μA/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 determination, etc. A team of professionals runs the facility and facilitates 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 other 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 ($C_s^+$, $O_2^+$). 1 μm resolution. |
| 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 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 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<br>Scintag diffractometers(2) | X-ray | 4-circle diffractometer. Small angle camera. EXAFS. Lang topography, Powder cameras, etc. High temperature and low temperature stages. Texture analysis. |
| 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 1.5MeV Kratos microscope dedicated largely to in situ work, a 1-MeV JEOL atomic resolution microscope (ARM) with 1.6 angstrom point-to-point resolution, 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 a parallel 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
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, ±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, intermediate 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 two 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, J. Bentley, C. B. Carter, B. Fabes, 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 Institute for Science and Education (ORISE).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik (615) 574-5066
Metals and Ceramics Division
Oak Ridge National Laboratory
P. O. Box 2008
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## 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 |
| 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 μm 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, on beam deposition 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 | 0.1-3.0 MeV; H, $^4$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; rf gas or sputtering source for up to 7 MeV ion beam of most element |
| 10-200-KV high-current ion implantation accelerator | Most ion species; 100-1000 microamps singly charged, microamps doubly and triply charged 10 |
| 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; PIXE; 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 to enhance the science and engineering of materials synthesis and processing in order to meet the programmatic needs of the Department of Energy and to facilitate the technological exploitation of 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. Emphasis the concurrent development of S&P by working with the DOE technologies and industry to advance processing science and its applications 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. Establish partnerships among the DOE Laboratories, Universities and Industry to capitalize on the *complementary strengths of these various institutions. The industrial connection is especially important* to shorten the time between the generation and application of MS&E knowledge and to enhance technology transfer.
5. Establish an Industrial Steering Group to provide the Center an industrial perspective on the selection of problems of potential commercial value.
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
Advanced 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, 1993, the Materials Sciences total support level amounted to about $270.0 million in operating funds (budget outlays) and $25.8 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) | 36.6 | 23.4 |
| (b) South................... (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV) | 11.0 | 19.2 |
| (c) Midwest................. (IA, IL, IN, MI, MN, MO, OH, WI) | 27.8 | 34.4 |
| (d) West.................... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA) | 24.6 | 23.0 |
| | 100.0 | 100.0 |

2. By Discipline:

| | Grant Research (% by $) | Total Program (% by $) |
|---|---|---|
| (a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-) | 62.2 | 49.2 |
| (b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-) | 27.2 | 21.5 |
| (c) Materials Chemistry (Budget Activity Numbers 03-) | 9.8 | 7.8 |
| (d) Facility Operations | — | 20.9 |
| | 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) | 21.1 |
| (b) DOE Laboratory Research Programs | 28.0 |
| (c) Major Facilities at DOE Laboratories | 49.4 |
| (d) Industry and Other | 1.5 |
| | 100.0 |

4. By Laboratory and Grant Research:

| | Total Program (%) |
|---|---|
| Ames Laboratory | 3.4 |
| Argonne National Laboratory | 22.0 |
| Brookhaven National Laboratory | 18.7 |
| Idaho National Engineering Laboratory | 1.5 |
| Illinois, University of (Materials Research Laboratory) | 2.7 |
| Lawrence Berkeley Laboratory | 13.9 |
| Lawrence Livermore National Laboratory | 0.8 |
| Los Alamos National Laboratory | 4.5 |
| National Renewable Energy Laboratory | 0.3 |
| Oak Ridge National Laboratory | 16.1 |
| Pacific Northwest Laboratory | 1.1 |
| Sandia National Laboratory | 2.9 |
| Stanford Synchrotron Radiation Laboratory | 1.0 |
| Grant Research | 11.1 |
| | 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 1993 were $270,225,000. The number of projects is 472.

## MATERIALS

Actinides-Metals, Alloys and Compounds

5, 15, 31, 32, 55, 133, 140, 158, 160, 175, 227, 240, 288, 334, 376, 403
(0.97, 0.47, 3.39)

Aluminum and its Alloys

8, 18, 41, 55, 67, 72, 81, 117, 140, 155, 169, 170, 176, 185, 220, 272, 273, 284, 308, 329, 339, 354, 360, 401, 445, 448, 449
(1.48, 0.51, 5.72)

Alkali and Alkaline Earth Metals and Alloys

4, 41, 61, 175, 274, 386, 448
(0.44, 0.20, 1.48)

Amorphous State: Liquids

38, 59, 105, 110, 136, 141, 195, 219, 261, 298, 300, 301, 352, 380, 399, 435
(0.93, 0.37, 3.39)

Amorphous State: Metallic Glasses

19, 23, 28, 70, 72, 117, 125, 141, 148, 154, 175, 185, 208, 219, 250, 294, 344, 416
(0.85, 0.66, 3.81)

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

29, 84, 90, 141, 151, 178, 181, 208, 219, 222, 223, 234, 253, 297, 301, 310, 350, 430
(0.76, 0.56, 3.81)

Amorphous State: Non-Metallic Glasses (Silicates)

16, 88, 201, 207, 219, 223, 225, 239, 253, 290, 297, 301, 310, 344, 391, 413, 420, 430, 439
(1.29, 0.37, 4.03)

Carbides

16, 80, 84, 119, 140, 143, 144, 177, 179, 192, 193, 223, 234, 257, 259, 266, 344, 354, 424, 438, 445
(0.89, 0.60, 4.45)

Cement and Concrete

369
(0.21, 0.03, 0.21)

Carbon and Graphite

57, 117, 131, 141, 185, 215, 216, 218, 252, 366, 386, 394
(0.64, 0.24, 2.54)

Coal

176
(0.02, 0.04, 0.21)

Composite Materials--Structural

3, 7, 13, 24, 119, 153, 171, 185, 199, 200, 223, 256, 259, 317, 327, 330, 354, 370, 418, 426, 439
(0.95, 0.55, 4.45)

Critical/Strategic Elements (Cr, Co, and Mn-Pt Alloys--use indexes below, also see Critical/Strategic Materials Substitution in the Phenomena Index.) Not to appear in Summary Book.

7, 306, 398, 456
(0.28, 0.08, 0.85)

Copper and its Alloys

2, 3, 7, 13, 27, 40, 41, 55, 69, 71, 75, 85, 95, 115, 143, 155, 166, 169, 187, 229, 231, 255, 289, 305, 314, 320, 329, 353, 384, 396, 432, 461
(1.57, 0.74, 6.78)

Dielectrics

14, 16, 90, 102, 130, 141, 177, 178, 179, 204, 215, 221, 271, 328, 367
(0.66, 0.32, 3.18)

Fast Ion Conductors (use Solid Electrolytes if more appropriate)

29, 41, 177, 178, 221, 222, 271, 319, 455
(0.44, 0.31, 1.91)

Iron and its Alloys

1, 2, 3, 6, 8, 15, 40, 52, 55, 56, 69, 71, 75, 79, 81, 85, 87, 95, 116, 138, 140, 155, 169, 170, 172, 175, 176, 183, 200, 202, 217, 226, 229, 231, 235, 249, 268, 272, 279, 283, 286, 309, 318, 331, 347, 359, 360, 364, 365, 374, 390, 398, 408, 425, 426, 445, 451, 461
(3.56, 1.45, 12.29)

Glasses (use terms under Amorphous State)

177, 225, 301, 310, 324, 371, 428, 439
(0.53, 0.10, 1.69)

Hydrides

20, 61, 81, 86, 176, 216, 250, 293, 374
(0.36, 0.27, 1.91)

## TECHNIQUES

Electron Spectroscopy for Chemical Analysis (ESCA)

30, 33, 41, 61, 77, 79, 81, 84, 97, 111, 119, 124, 139, 141, 144, 155, 178, 266, 323, 366, 455
(0.61, 0.41, 4.45)

Electron Spin Resonance or Electron Paramagnetic Resonance

39, 89, 120, 125, 163, 179, 212, 213, 271, 281, 318, 326, 375
(0.51, 0.43, 2.75)

Extended X-Ray Absorption Fine Structure (EXAFS and XANES)

32, 33, 40, 51, 52, 63, 84, 88, 132, 139, 150, 219, 227, 266, 273, 275, 291, 350, 351, 355, 382, 430, 431, 432, 451, 452, 453
(1.12, 0.61, 5.72)

Field Emission and Field Ion Microscopy

22, 24, 74, 167, 168, 206, 211, 352
(0.38, 0.31, 1.69)

High Pressure (Technique development of all types)

12, 29, 40, 130, 158, 159, 161, 163, 195, 213, 253, 275
(0.44, 0.35, 2.54)

Ion or Molecular Beams

23, 39, 41, 42, 70, 77, 94, 97, 102, 120, 142, 161, 165, 167, 170, 181, 189, 190, 214, 229, 242, 251, 289, 359
(1.04, 0.72, 5.08)

Ion Channeling, or Ion Scattering (including Rutherford and other ion scattering methods)

23, 26, 28, 41, 70, 73, 81, 94, 120, 146, 152, 167, 170, 178, 179, 190, 191, 208, 226, 242, 243, 321, 366, 420
(1.12, 1.34, 5.08)

Internal Friction (also see Ultrasonic Testing and Wave Propagtion)

154, 271, 278
(0.04, 0.02, 0.64)

Infrared Spectroscopy (also see Raman Spectroscopy)

39, 40, 89, 126, 129, 144, 159, 163, 177, 178, 181, 201, 207, 208, 215, 218, 222, 225, 266, 271, 275, 296, 319, 323, 345, 423, 462
(1.33, 0.54, 5.72)

Laser Spectroscopy (scattering and diagnostics)

41, 42, 122, 128, 129, 130, 135, 136, 137, 141, 151, 159, 165, 181, 195, 199, 203, 204, 209, 210, 214, 215, 218, 261, 285, 290, 297, 342, 346, 348, 380, 381, 385, 399, 417, 433, 439, 441, 457
(1.93, 0.76, 8.26)

Magnetic Susceptibility

5, 12, 13, 25, 30, 31, 34, 37, 54, 92, 125, 145, 152, 158, 161, 162, 180, 189, 212, 213, 240, 262, 288, 292, 318, 326, 375, 398, 429
(1.80, 1.03, 6.14)

Molecular Beam Epitaxy

30, 76, 77, 94, 97, 98, 99, 100, 102, 120, 137, 141, 165, 181, 182, 188, 209, 210, 226, 241, 248, 291, 295, 431
(1.04, 0.45, 5.08)

Mössbauer Spectroscopy

31, 39, 187, 249, 343, 378, 411, 440, 451, 453
(0.81, 0.23, 2.12)

Neutron Scattering: Elastic (Diffraction)

11, 14, 29, 34, 37, 38, 39, 55, 56, 57, 62, 92, 105, 155, 158, 161, 163, 175, 176, 183, 189, 194, 198, 203, 248, 250, 301, 319, 362, 394, 414, 435, 453, 464, 466, 469
(1.67, 2.87, 7.63)

Neutron Scattering: Inelastic

11, 29, 34, 38, 39, 55, 56, 62, 92, 105, 163, 175, 176, 194, 198, 248, 265, 308, 378, 394, 414, 434, 435, 440, 464, 466, 469
(1.55, 2.58, 5.72)

Neutron Scattering: Small Angle

29, 34, 39, 143, 174, 176, 194, 197, 198, 217, 302, 325, 365, 414, 424, 435, 464, 466, 469, 472
(1.25, 2.19, 4.24)

Nuclear Magnetic Resonance and Ferromagnetic Resonance

12, 39, 89, 106, 123, 125, 135, 143, 144, 199, 212, 222, 225, 252, 266, 271, 296, 302, 310, 382, 391, 423, 447
(1.48, 0.58, 4.87)

Optical Absorption

15, 22, 33, 39, 112, 122, 128, 141, 151, 163, 178, 181, 204, 210, 218, 290, 304, 348, 471
(0.70, 0.35, 4.03)

Perturbed Angular Correlation and Nuclear Orientation

382
(0.06, 0.01, 0.21)

Photoluminescence

16, 99, 110, 128, 141, 151, 161, 165, 181, 210, 218, 290, 297, 334, 367, 436, 437
(0.72, 0.28, 3.60)

Positron Annihilation (including slow positrons)

59, 63, 67, 332
(0.15, 0.14, 0.85)

Powder Consolidation (including sintering, hot pressing, dynamic compaction, laser assisted, etc., of metals and ceramics, use this item in the Phenomena index)

7, 10, 27, 54, 90, 93, 119, 139, 154, 161, 171, 180, 189, 199, 259, 278, 286, 319, 347, 426, 439
(1.10, 0.70, 4.45)

Theory: Defects and Radiation Effects

26, 35, 53, 67, 68, 70, 94, 147, 149, 152, 157, 163, 170, 186, 202, 227, 234, 251, 271, 280, 293, 321, 342, 350, 367
(1.23, 2.18, 5.30)

Theory: Electronic and Magnetic Structure

5, 19, 25, 33, 34, 35, 39, 40, 50, 60, 92, 101, 115, 131, 140, 141, 149, 157, 158, 160, 163, 166, 169, 186, 204, 210, 212, 216, 217, 223, 228, 245, 263, 281, 287, 288, 290, 293, 295, 334, 340, 341, 344, 376, 378, 379, 383, 397, 403, 440, 443, 447
(2.67, 1.22, 11.02)

Theory: Non-Destructive Evaluation

8, 232
(0.15, 0.05, 0.42)

Theory: Surface

34, 35, 41, 50, 60, 68, 74, 91, 101, 121, 124, 131, 132, 136, 144, 157, 165, 166, 169, 182, 186, 201, 206, 216, 237, 247, 255, 294, 295, 316, 333, 349, 357, 370, 372, 395, 397, 400, 420, 443, 459
(2.48, 1.03, 8.69)

Theory: Structural Behavior

4, 5, 18, 86, 104, 105, 115, 119, 131, 157, 165, 166, 171, 173, 207, 230, 256, 257, 270, 272, 274, 276, 278, 293, 295, 317, 322, 328, 330, 331, 333, 334, 337, 339, 346, 353, 354, 356, 364, 370, 372, 383, 394, 396, 404, 416, 418, 419, 420, 424, 443, 449, 450, 457
(4.62, 1.24, 11.44)

Theory: Superconductivity

17, 27, 31, 34, 53, 60, 101, 123, 125, 131, 157, 158, 161, 186, 189, 212, 228, 288, 328, 344, 356, 376, 429, 444, 447
(1.50, 0.79, 5.30)

Theory: Thermodynamics, Statistical Mechanics, and Critical Phenomena

38, 50, 60, 101, 104, 105, 115, 125, 135, 140, 148, 154, 157, 162, 165, 166, 171, 181, 186, 194, 195, 196, 197, 216, 225, 230, 231, 239, 244, 245, 255, 270, 272, 274, 281, 287, 293, 294, 313, 324, 328, 333, 409, 436, 437, 453, 461
(2.39, 1.15, 9.96)

Theory: Transport, Kinetics, Diffusion

1, 2, 25, 39, 40, 53, 69, 70, 74, 86, 138, 141, 142, 143, 169, 170, 181, 182, 186, 195, 198, 210, 216, 230, 233, 234, 239, 244, 245, 263, 271, 278, 280, 293, 294, 319, 323, 328, 335, 338, 344, 360, 362, 371, 379, 383, 388, 389, 390, 397, 399, 403, 406, 409, 419, 420, 425, 472
(3.16, 2.65, 12.29)

Thermal Conductivity

162, 198, 428
(0.21, 1.45, 0.64)

Ultrasonic Testing and Wave Propagation

8, 69, 154, 308
(0.21, 0.07, 0.85)

## ENVIRONMENT

## MAJOR FACILITIES: OPERATIONS

Pulsed Neutron Sources (Operations)

45, 156, 164, 464, 466, 469
(0.95, 5.40, 1.27)

Steady State Neutron Sources (Operations)

64, 198, 414, 464, 466, 469
(0.95, 16.93, 1.27)

Synchrotron Radiation Sources (Operations)

32, 40, 43, 65, 124, 127, 187, 206, 219, 273, 334, 452, 465
(2.54, 8.37, 2.75)

UNITED STATES DEPARTMENT OF ENERGY
ER-13
WASHINGTON, DC 20585

OFFICIAL BUSINESS