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Materials Sciences Programs

Fiscal Year 1991

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 structure of the Division is given in an accompanying chart.

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

This report contains a listing of research underway in FY 1991 together with a convenient index to the Division's programs. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page.

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

PUBLICATION REFERENCES

The Materials Sciences program has sponsored various workshops, topical and descriptive reports and co-sponsored Research Assistance Task Forces on select topics over the past 12 years. It is our intention to make as much as possible of the proceedings of these activities publically available through publication in open literature scientific journals, bulletins, or other archival forms. Many of these publications identify the authors perceptions of emerging or existing generic materials science research needs and opportunities. Their primary purpose is to stimulate creative thinking and new ideas by scientists within their respective topical fields. None of these publications, however, is intended to be all inclusive or to encompass with thoroughness any given topic, and none of them represents Department of Energy (DOE) policy or opinion. No pretense is made to have covered every materials science topic of interest in this listing, and the fact that there is no publication corresponding to a particular materials science topic does not, of itself, carry any implication whatsoever with respect to DOE interest or lack thereof. We have also included in this list the tentative title of those publications that we anticipate will be published over the next year, so as to alert our community to this likelihood.

"Deformation and Fracture of Intermetallics," M. H. Yoo, S. L. Sass, C. L. Fu, M. J. Mills, D. M. Dimiduk, E. P. George, to be submitted for publication

"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 - An Assessment Based on a Workshop Meeting," D. R. Clarke, et al., submitted for publication to J. Amer. Ceramic Soc.

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

"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, T. O. Mason, H. L. Tuller, and A. N. Cormack, to be submitted for publication

"Materials for Intelligent Systems," D. Smyth, R. E. Newnham, et al., to be submitted for publication

"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 Workshop," D. W. Keefer, S. A. David and H. Smartt, to be submitted for publication

"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

"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 1991 funding level, title, personnel, budget activity number (e.g., 01-2) and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), Materials Chemistry (03), or Facility Operations (04). The budget numbers carry the following titles:

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

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

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

04-1 - Facility Operation

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

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

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

Preparation of this FY 1991 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 Goodrich.

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SECTION A

Laboratories

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

AMES LABORATORY

Iowa State University
Ames, IA 50011

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

Metallurgy and Ceramics - 01 -

O. Buck - (515) 294-4446

1. ANALYSIS OF INTERFACES
A. J. Bevolo, J. D. Verhoeven
(515) 294-5414   01-1 $154,000

Studies of interface structure and composition using Auger, EELS, and SIMS surface analytical techniques in combination with ion etching. Auger and reflection electron loss spectroscopy of metallic hydrides for phase identification and mapping. Scanning Auger microprobe analysis of grain boundary segregation in irradiated steels, cast irons, V-Ti based alloys, and high-T_c superconductors. Local chemical state information from Auger lineshape analysis. Electronic structure of heavy fermion metals and binary transition metal alloys. Surface segregation in Ni and Pd based binary transition metal solid-solution alloys.

2. SOLIDIFICATION MICROSTRUCTURES
R. K. Trivedi, I. E. Anderson, L. S. Chumbley, R. W. McCallum, J. D. Verhoeven
(515) 294-5869   01-1 $173,000

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 napthalene. Directional solidification studies on segregation and morphology in gray, nodular, and white cast iron. Solidification processing of (Dy,Tb)Fe_2 magnetostrictive alloys, Nd-Fe-B permanent magnet materials, and intermetallic compounds, and analysis of their magnetic and mechanical properties.

3. CONTROLLED MICROSTRUCTURES
J. D. Verhoeven, A. J. Bevolo
(515) 294-9471   01-1 $311,000

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.

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

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

5. MECHANICAL BEHAVIOR OF MATERIALS
W. A. Spitzig, B. Biner, J. Kameda
(515) 294-5082   01-2 $388,000

Studies of the effects of environment and stress on the mechanical properties of metals, intermetallics, and ceramic composites. Effects of hydrogen on cracking in alloys under uniaxial and cyclic loading conditions. Interstitial effects on strength and ductility in both nonhydrogenated and hydrogenated V, Nb, and Ta. High-temperature-induced intergranular cracking in Ni base alloys. Effects of radiation-induced defects and solute segregation on intergranular embrittlement. Modeling of hydrogen embrittlement. Description of three dimensional arrays of defects and relationship of arrangement to ductility and mechanical properties. Correlation between defect structure and nondestructive measurement.

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

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

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

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

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

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

9. ADVANCED MATERIALS AND PROCESSES
F. A. Schmidt, I. E. Anderson, T. A. Lograsso, R. K. Trivedi, J. D. Verhoeven
(515) 294-5236 01-5 $570,000

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

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

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

Solid State Physics - 02 -

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

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

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

12. NEW MATERIALS AND PHASES
F. Borsa, R. G. Barnes, D. C. Johnston,
C. A. Swenson, D. R. Torgeson
(515) 294-5435 02-2 $590,000

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

13. SUPERCONDUCTIVITY
D. K. Finnemore, J. E. Ostenson
(515) 294-3455 02-2 $400,000

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 $270,000

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

15. OPTICAL, SPECTROSCOPIC, AND SURFACE PROPERTIES OF SOLIDS
D. W. Lynch, C. G. Olson, M. Tringides
(515) 294-3476 02-2 $525,000

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

16. SEMICONDUCTOR PHYSICS
H. R. Shanks, J. Shinar
(515) 294-8706 02-2 $270,000

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

17. SUPERCONDUCTIVITY THEORY
J. R. Clem, V. Kogan
(515) 294-4223 02-3 $169,000

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

18. OPTICAL AND SURFACE PHYSICS THEORY
R. Fuchs, C. T. Chan, K.-M. Ho
(515) 294-1960 02-3 $140,000

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

19. ELECTRONIC AND MAGNETIC PROPERTIES
B. N. Harmon, C. T. Chan, K.-M. Ho, M. Luban, C. Soukoulis
(515) 294-7712   02-3 $482,000

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

Materials Chemistry - 03 -

P. A. Thiel - (515) 294-2770

20. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS
J. D. Corbett, R. A. Jacobson, R. E. McCarley
(515) 294-3086   03-1 $550,000

Synthesis, structure and bonding in intermetallic systems--new Zintl phases, new ternary compounds stabilized by interstitials. The effect of common imparities on stability. Systematic variation of conduction, magnetic, and corrosion resistance properties. 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. Development of diffraction techniques for single crystal and non-single crystal specimens, techniques for pulsed-neutron and synchrotron radiation facilities, and use of Patterson superposition methods. Experimental methods include X-ray diffraction, photoelectron spectroscopy, resistivity and magnetic susceptibility measurements, high temperature reactions and synthesis of molecular precursors.

21. CERAMICS AND POLYMERS
T. J. Barton, M. Akinc, K. Woo
(515) 294-2770   03-2 $382,000

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. Polymers containing transition metal arrays.

22. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS
H. F. Franzen, J. W. Anderegg
(515) 294-5773   03-3 $246,000

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

23. SURFACE CHEMISTRY
P. A. Thiel, K. G. Baikerikar, R. S. Hansen, D. C. Johnson
(515) 294-8985   03-3 $546,000

Study of lubrication phenomena: decomposition pathways and products of fluorinated ethers at surfaces. Mechanisms of oxidation of metals; formation of thin, metastable oxide overlayers. Mechanisms of oxidative corrosion of metals.

Chemistry of electrode reactions, including electrocatalysis and corrosion reactions. Characterization of electrocatalytic materials by modulated hydrodynamic voltammetry. Reactivity of oxidized and doped electrode surfaces, including characterization of oxygen mobility and defect density at such electrodes. Surface chemistry of nucleation and flocculation applied to ceramic processing. Techniques used include low energy electron diffraction, Auger electron spectroscopy, electron energy loss spectroscopy, temperature programmed desorption, electron-stimulated desorption, ring-disk and modulated hydrodynamic voltammetry.

ARGONNE NATIONAL LABORATORY

9700 South Cass Avenue
Argonne, IL 60439

F. Y. Fradin - (708) 252-3504/FTS 252-3504

Metallurgy and Ceramics - 01 -

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

24. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH
N. J. Zaluzec, C. W. Allen
(708) 252-5075 01-1 $1,614,000

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 (1300K), cooling (10K), straining, resistivity and gaseous environments. Ion-beam interface with 650 kV ion accelerator and 2 MV tandem accelerator available for in situ implantations and irradiations. Approximately 50 percent of HVEM usage is by non-ANL scientists on research proposals approved by the Steering Committee for the Center that meets every 6 months. A state-of-the-art, medium-voltage, ultra-high vacuum, field-emission gun, Analytical Electron Microscope is being procured. Its design is directed toward the attainment of the highest microanalytical resolution and sensitivity. Fundamental studies of electron-solid interactions and microcharacterization of materials, using TEM, STEM, XEDS, and EELS are conducted at present on conventional transmission electron microscopes (JEOL 4000 EXII, JEOL 100CX, Philips EM420, and Philips CM30).

25. BASIC CERAMICS
D. J. Lam, S.-K. Chan, S. J. Rothman, J. L. Routbort, B. W. Veal
(708) 252-4966 01-3 $1,292,000

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

26. INTERFACE STUDIES
K. L. Merkle, J. N. Mundy
(708) 252-4990 01-3 $710,000

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.

27. 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 $1,510,000

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

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

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

29. AMORPHOUS AND NANOCRYSTALLINE MATERIALS
L. E. Rehn, J. Eastman, P. R. Okamoto, R. W. Siegel (708) 252-4963
(708) 252-5021 01-5 $684,000

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. Mechanical properties and sintering characteristics of nanocrystalline ceramics and metals. Synthesis of ultra-fine metallic powders. Materials characterization methods include X-ray and neutron diffraction, electron microscopy, electrical resistivity, Rutherford backscattering, AES, EELS, and EXAFS.

Solid State Physics - 02 -

B. D. Dunlap - (708) 972-4925

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30. NEUTRON AND X-RAY SCATTERING
J. D. Jorgensen, J. E. Epperson, G. P. Felcher, R. Kleb, D. L. Price, S. Susman
(708) 252-5513 02-1 $1,632,000

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

31. TWO-DIMENSIONAL MATERIALS
S. D. Bader, M. B. Brodsky, M. Grimsditch, C. Liu
(708) 252-4960 02-2 $863,000

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

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

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

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

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

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

The group is involved in experimental studies using synchrotron radiation techniques of the electronic and structural properties of materials. X-ray absorption techniques has been employed in the study of the valence state of a diverse number of compounds, i.e., high-T_c superconductors. An X-ray scattering beam line has been developed at one of the national synchrotron sources for the study of interfaces using X-ray scattering techniques. An X-ray photoelectron microscope was developed with high spatial resolution using the group's soft X-ray beam line at Wisconsin. Angle resolved photoemission spectroscopy has been used to fundamental properties of high-T_c superconductors. In situ X-ray scattering has been used in the characterization of the structure of electrochemical interfaces. Thin film growth and interface composition have been investigated using X-ray reflectivity techniques.

35. CONDENSED MATTER THEORY
D. D. Koelling, A. A. Abrikosov, R. Benedek, M. Norman, M. Randeria, K. J. Strandburg, N. Trivedi
(708) 252-5507 02-3 $1,127,000

Condensed matter theory in statistical physics, electronic band theory, and many body effects. Possible non-Fermi liquid behavior in two dimensional systems. Quasicrystal structure and interface roughening. Coarsening in cellular networks (e.g., grain growth). Monte Carlo methods. Electronic structure calculations of narrow band metal and alloy systems. Correlation effects in narrow band metals and metal oxide insulators. Monte Carlo studies of fractional quantum Hall states. Large-cell electronic structure and cohesive property calculations. Photoemission lineshape spectra for complex materials. Positron annihilation effects in metals and alloys. Studies of the new high-T_c superconductors. Superconductivity in heavy fermion metals. Magnetic quantization effects in superconductors. Raman continuum in layered superconductors. Phenomenological studies of the mixed state in layered superconductors. Vortex structure in layered superconductors.

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

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

37. ULTRA-HIGH FIELD SUPERCONDUCTORS
K. E. Gray, R. T. Kampwirth
(708) 252-5525 02-5 $369,000

Emphasis is on the development of a low-temperature, high-rate sputtering process for the new high-temperature, high-field oxide superconductors. Films of the YBa_2CuO_7, Bi-Sr-Ca-Cu-O and Tl-Ba-Ca-Cu-O systems have been successfully made using conventional high-temperature annealing, and new low-temperature in situ techniques are being investigated. The effort includes the effects of preparation conditions, substrate type, annealing steps and target composition on the superconducting properties. Material characterization by X-ray, SEM, TEM, RBS, ICPAES and superconducting properties. Layered NbN/AlN films exhibiting 4-5 times higher critical current density than NbN at high fields will also be addressed.

Materials Chemistry - 03 -

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

38. CHEMICAL AND ELECTRONIC STRUCTURE
J. M. Williams, K. D. Carlson, G. M Frankenbach, U. Geiser, A. M. Kini, A. J. Schultz, H. H. Wang
(708) 252-3464 03-1 $1,424,000

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 (10-300K) using the IPNS-SCD and a low-temperature (10K) single crystal X-ray diffraction instrument.

39. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS
M. Blander, L. A. Curtiss, M.-L. Saboungi
(708) 252-4548 03-2 $413,000

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.

40. INTERFACIAL MATERIALS CHEMISTRY
V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, A. R. Krauss
(708) 252-4547 03-2 $499,000

Basic research on interfacial phenomena in two forefront scientific fields of materials science: (1) molecular sieve materials and their application in heterogeneous catalysis and (2) novel techniques for the preparation and characterization of high-critical-temperature (T_c) superconductors in thin-film form. 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 cataylsts and template effects in microporous structure development. Production and characterization of multicomponent thin films and layered structures by computer-controlled sequential deposition with in situ annealing and oxidation processes as part of an integrated fabrication cycle. Use of ozone, atomic oxygen, and oxygen ion beam modification to produce high temperature superconductor (HTSC) films with little or no high temperature annealing. Atomic layer-by-layer fabrication of Bi based HTSCs. Production of superlattice structures for electronic applications and thin-film optoelectronic devices. Basic surface studies of as-grown superconducting thin films; basic studies of growth processes for multicomponent thin films.

41. AQUEOUS CORROSION
V. A. Maroni, L. A. Curtiss, C. A. Melendres, Z. Nagy, R. M. Yonco
(708) 252-4547 03-2 $644,000

Basic research aimed at elucidating fundamental aspects of aqueous corrosion under conditions of temperature and pressure (300°C and 10 MPa) relevant to light water fission reactor environments.

Investigations of the mechanisms responsible for passivation on iron, copper, and nickel-based alloys and for crack and pit propagation in these same alloys. Studies of the details that connect surface adsorption, electron transfer, and electrolyte chemistry with passive film structure using a combination of in situ surface sensitive spectroscopic methods and transient electrochemical techniques. In situ characterization of metal/solution interfaces using laser Raman, photoelectrochemicals and X-ray spectroscopies. Investigations of the key features of the interfacial chemistry associated with passivation processes (including charge transfer kinetics and film-growth dynamics) using pulsed galvanostatic, potentiostatic, dc polarization, and ac impedance through the application of molecular dynamics methods in combination with ab initio molecular orbital theory.

42. PARTICLE AND PHOTON INTERACTIONS WITH SURFACES
D. M. Gruen, W. F. Calaway, A. R. Krauss, G. J. Lamich, M. J. Pellin, C. E. Young
(708) 252-3513 03-3 $1,028,000

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.

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

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

Facility Operations - 04 -

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

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44. INTENSE PULSED NEUTRON SOURCE PROGRAM
B. S. Brown, J. M. Carpenter, R. K. Crawford, J. Richardson, F. J. Rotella, A. W. Schulke, P. Thiyagarajan, F. Trouw, T. G. Worlton
(708) 252-4999 04-1 $6,221,000

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 one instrument under construction. The facility has been run since 1981 as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 320 experiments, involving about 150 outside visitors from universities and other institutions are performed annually. Industrial Research on a proprietary basis, which allows the company to retain full patent rights, has been initiated with a number of companies (e.g., DuPont, 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. An enriched uranium target was installed in 1988 that increased the flux by a factor of 2.5.

45. APS ACCELERATOR R&D
Y. Cho, E. Crosbie, G. Decker, J. Galayda, G. Goeppner, J. Howell, J. Jagger, M. Knott, R. Kustom, G. Mavrogenes, D. McGhee, J. Noonan, A. Passi, L. Teng
(708) 252-6616 04-1 $9,153,000

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

46. APS BEAMLINE AND INSERTION DEVICE R&D
G. K. Shenoy, E. E. Alp, S. H. Barr, D. Carnegie, E. Gluskin, A. Khounsary, D. M. Mills, R. K. Smither, P. J. Viccaro, W. Yun
(708) 252-5537 04-1 $4,768,000

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

BROOKHAVEN NATIONAL LABORATORY
Upton, NY 11973

J. D. Axe - (516) 282-3821/FTS 666-3821

Metallurgy and Ceramics - 01 -

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

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

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

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

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

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

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

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

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

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

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

Solid State Physics - 02 -

M. Strongin - (516) 282-3763

52. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES
S. M. Shapiro, A. Gibaud, L. Passell, L. Rebelsky
(516) 282-3822 02-1 $1,380,000

This program is directed to the study of elementary excitations in condensed matter and to the development of new neutron scattering techniques to further these investigations. Currently, experimental interest focuses on excitations in heavy fermion, mixed valent and paramagnetic systems, on magnetism in graphite intercalation compounds, and on the structures and dynamical response of adsorbed gas films. 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 beam line and tests made of its performance. It is expected to be in routine operation within the year. This, as well as other recently completed projects and such continuing projects as the United States-Japan (U.S.-Japan) collaborative research program, represent a significant expansion of the condensed matter research capability of the HFBR. Part of the effort in new instrument development will also contribute to the Advanced Neutron Source Project at Oak Ridge National Laboratory.

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

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

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

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

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

The objective of this program is to exploit the technique of synchrotron X-ray scattering to study structure and magnetism in solids and complex fluids. Emphasis is given to studies of the structure and phase behavior of surfaces, interfaces, and thin films utilizing a UHV X-ray scattering chamber and special X-ray cells for studying scattering from solid/liquid and liquid/vapor interfaces. A new direction has involved studies of surfaces under electrochemical conditions. Magnetic structure is probed via magnetic X-ray scattering, particularly resonant magnetic scattering.

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

Perfect and imperfect solids, solid and liquid interfaces and their surfaces are investigated by newly developed experimental methods using variable energy positron (.1 eV - 3 MeV) and positronium beams coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron Diffraction, and Thermal Desorption Spectroscopy). These methods include two-dimensional angular correlation of annihilation radiation, positronium scattering positron induced Auger Electron Spectroscopy, positron channeling and diffusion lengths, positron work functions, and positronium formation with measurement of its emitted energy distribution on surfaces. Systems that are being studied include metal-metal, and oxide-semiconductor and metal-semiconductor interfaces and their alloy formation. Bulk positron lifetime and Doppler broadening measurements are being performed on various systems including high temperature superconductors and some metallic alloys. Improved modeling of positron implantation and diffusion in homogeneous and layered solids through Monte Carlo simulation is being developed to carry out quantitative depth profiling.

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

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

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

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

Materials Chemistry - 03 -

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

The study of phase transitions and critical phenomena on surfaces in a wide variety of materials, forms the framework of the neutron scattering program. Recent work centers around the structure and dynamics of rare gas and hydrocarbon films on graphite and the layer-by-layer growth and melting of these films. In addition, efforts to image Rayleigh-Benard convective flows in liquid helium mixtures and to synthesize materials with novel physical properties continues. The combination of elastic, absorptive, and inelastic neutron techniques presents a method unrivaled in its ability to render a microscopic view of a wide range of physical phenomena. These experiments provide needed data for the testing, and possible modification, of theoretical models.

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

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

Facility Operations - 04 -

M. Brooks - (516) 282-4061

61. EXPERIMENTAL RESEARCH- HIGH FLUX BEAM REACTOR - OPERATIONS
M. H. Brooks, W. Brynda, J. Detweiler, O. Jacobi, J. Junker, V. Lettieri, J. Petro, T. Prach, R. Reyer, D. C. Rorer, P. Tichler
(516) 282-4061 04-1 $24,809,000

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

62. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT

D. B. McWhan, I. Ben-Zvi, A. M. Fauchet, J. Godel, J. Hastings, R. Heese, R. Klaffky, S. Krinsky, D. P. Siddons, W. Thomlison, G. P. Williams
(516) 282-3927 04-1 $15,910,000

This program supports the operation of the National Synchrotron Light Source (NSLS), which is a large user facility devoted to the production and utilization of synchrotron radiation, and it supports the development of electron based radiation sources and 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 beam lines on the vacuum ultraviolet (VUV) and X-ray storage rings. As this is the first facility in the U.S. that was designed expressly for the use of synchrotron radiation, there are extensive development programs to improved the stability, reliability, and lifetime of electron beams and to develop new insertion devices which give even brighter photon beams. Equally important are programs to develop new beam line inestrumentation including beam line optics, monochromators and detectors which will permit users to take full advantage of the unique research capabilities offered by the NSLS. Finally, substantial maintenance, upgrade, and safety programs are required for the operation of the facility.

IDAHO NATIONAL ENGINEERING LABORATORY
Idaho Falls, ID 83415

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

Metallurgy and Ceramics - 01 -

D. W. Keefer - (208) 526-8003

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

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

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

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

UNIVERSITY OF ILLINOIS MRL

104 S. Goodwin Avenue
Urbana, IL 61801

H. Birnbaum - (217) 333-1370

Metallurgy and Ceramics - 01 -

H. Birnbaum - (217) 333-1370

65. THEORY OF DEFECTS AND INTERFACES IN BCC METALS
J. Adams
(217) 244-7709 01-1 $83,578

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

66. TRANSPORT PROCESSES IN LOCALIZED CORROSION
R. C. Alkire
(217) 333-3640 01-1 $128,620

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

67. DEFECTS, DIFFUSION, AND NONEQUILIBRIUM PROCESSING OF MATERIALS
R. S. Averback
(217) 333-4302 01-1 $230,126

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

68. MOLECULAR SPECTROSCOPY OF THE SOLID-LIQUID INTERFACE
P. W. Bohn
(217) 333-0676 01-1 $58,212

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

69. CENTER FOR MICROANALYSIS OF MATERIALS
J. A. Eades, C. Loxton
(217) 333-8396 01-1 $75,060

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

70. MICROANALYSIS OF DEFECTS AND INTERFACES
J. A. Eades
(217) 333-8396 01-1 $137,149

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

71. ATOMISTICS OF GROWTH AND TRANSPORT AT METAL AND SEMICONDUCTOR INTERFACES
G. Ehrlich
(217) 333-6448 01-1 $145,646

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

72. ATOMIC RESOLUTION ELECTROCHEMISTRY OF CORROSION AND DEPOSITION PROCESSES
A. A. Gewirth
(217) 333-8329 01-1 $60,825

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

73. TRANSMISSION ELECTRON MICROSCOPY OF SURFACES AND INTERFACES
J. M. Gibson
(217) 333-2997 01-1 $129,940

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.

74. CHEMISTRY OF NEW TRANSITION METAL CERAMIC COMPOUNDS SYNTHESIZED BY MOCVD
G. S. Girolami
(217) 333-2729 01-1 $89,143

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.

75. CRYSTAL GROWTH AND PHYSICAL PROPERTIES OF METASTABLE SEMICONDUCTING, CERAMIC AND METALLIC ALLOYS
J. E. Greene
(217) 333-0747 01-1 $166,175

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

76. ORGANIZATION OF THE SINGLE-CRYSTAL SOLID-LIQUID INTERFACE: ENERGIES, STRUCTURES AND ELECTRONIC SYNERGISM
A. Wieckowski
(217) 333-7943 01-1 $61,207

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

77. MICROSTRUCTURE EVOLUTION, INTERFACES AND PROPERTIES IN STRUCTURAL CERAMIC COMPOSITES
A. Zangvil
(217) 333-6829 01-1 $171,319

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.

78. MECHANISMS OF ENVIRONMENTALLY INDUCED EMBRITTLEMENT
C. J. Altstetter
(217) 333-4985 01-2 $91,361

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

79. SOLUTE EFFECTS ON MECHANICAL PROPERTIES OF GRAIN-BOUNDARIES
H. K. Birnbaum
(217) 333-1370 01-2 $261,502

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.

80. COUNCIL ON MATERIALS SCIENCE
C. P. Flynn
(217) 333-1370 01-2 $117,940

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.

81. MECHANICAL PROPERTIES OF INTERMETALLIC COMPOUNDS
C. Loxton, I. M. Robertson
(217) 333-0386 01-2 $213,403

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

82. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF CERAMICS
D. F. Socie
(217) 333-7630 01-2 $90,910

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.

83. SUBCRITICAL CRACK GROWTH IN STRUCTURAL CERAMICS
J. F. Stubbins
(217) 333-6474 01-2 $80,884

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.

84. STRUCTURE AND KINETICS OF ORDERING TRANSFORMATIONS IN METAL ALLOYS AND SILICIDE THIN FILMS
H. Chen
(217) 333-7636 01-3 $125,702

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.

85. MATERIALS CHEMISTRY OF OXIDES CERAMICS; FIELD RESPONSIVE OGRANIC INCLUSION COMPLEXES
W. F. Klemperer
(217) 333-2995 01-3 $283,271

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.

86. SYNTHESIS AND PROPERTIES OF ELECTRICAL CERAMICS
D. A. Payne
(217) 333-2937 01-3 $368,265

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.

87. ATOMIC SCALE MECHANISMS OF VAPOR PHASE CRYSTAL GROWTH
A. Rockett
(217) 333-0417 01-3 $102,376

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

88. PROCESSING OF MONODISPERSE CERAMIC POWDERS
C. Zukoski
(217) 333-7379 01-3 $277,386

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.

89. ULTRASONIC STUDIES OF DEFECTS IN GaAs
A. W. Granato
(217) 333-2639 01-4 $37,272

Elastic and anelastic studies of defects in GaAs. Correlation with electronic properties of deep lying defect levels.

90. RADIATION EFFECTS IN METALS AND SEMICONDUCTORS
I. M. Robertson
(217) 333-6776 01-4 $95,000

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

Solid State Physics - 02 -

H. Zabel - (217) 333-2514

91. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS
A. C. Anderson
(217) 333-2866 02-2 $104,023

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

92. SYNTHESIS AND CHARACTERIZATION OF ORGANOMETALLIC LIQUID CRYSTAL POLYMERS
T. L. Brown
(217) 244-1176 02-2 $50,042

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

93. ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES
T.-C. Chiang
(217) 333-2593 02-2 $154,209

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.

94. THEORY OF SOLIDS, SURFACES AND HETEROSTRUCTURES
R. M. Martin
(217) 333-4229 02-2 $111,457

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.

95. GROWTH AND PROPERTIES OF NOVEL MBE STRUCTURES II. SEMICONDUCTOR HETEROSTRUCTURES
H. Morkoc, C. P. Flynn
(217) 333-0722 02-2 $301,611

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

96. DESIGN AND SYNTHESIS OF NEW ORGANOMETALLIC MATERIALS
T. B. Rauchfuss
(217) 333-7355 02-2 $124,647

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. Synthesis of metal clusters containing reactive ester groups will be developed for the applications to organometallic polyesters. The reactivity inherent in main group vertices of metal clusters will be used to generate clusters-of-clusters. Synthetic studies will focus on charge transfer salts containing organometallic donors and acceptors.

97. PROPERTIES OF CRYSTALLINE AND LIQUID CONDENSED GASES
R. O. Simmons
(217) 333-4170 02-2 $178,711

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.

98. NUCLEAR MAGNETIC RESONANCE IN SOLIDS
C. P. Slichter
(217) 333-3834 02-2 $218,558

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.

99. ELECTRO-ACTIVE AND NONLINEAR OPTICAL POLYMERS
S. I. Stupp
(217) 333-4436 02-2 $148,360

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.

100. METALLOPORPHYRINS AS FIELD RESPONSIVE MATERIALS
K. S. Suslick
(217) 333-2794 02-2 $57,149

The synthesis and characterization of porphyrinic 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.

101. CARRIER TRANSPORT IN QUANTUM WELLS - PICOSECOND IMAGING
J. P. Wolfe
(217) 333-2374 02-2 $106,176

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.

102. STRUCTURE AND DYNAMICS OF SURFACES, INTERFACES AND HETEROSTRUCTURES
H. Zabel
(217) 333-2514 02-2 $74,983

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

Materials Chemistry - 03 -

H. Zabel - (217) 333-2514

103. HIGH PRESSURE STUDIES OF MOLECULAR AND ELECTRONIC PHENOMENA
H. G. Drickamer
(217) 333-0025   03-1 $176,051

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.

104. SURFACE STUDIES OF BOUNDARY LAYER FILMS
A. J. Gellman
(217) 244-5810   03-1 $46,302

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

105. MECHNISTIC AND SYNTHETIC STUDIES IN CHEMICAL VAPOR DEPOSITION
R. G. Nuzzo
(217) 244-0809   03-1 $44,521

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.

106. OPTICAL SPECTROSCOPY OF SURFACE PROCESSES IN THIN FILM DEPOSITION
E. G. Seebauer
(217) 333-4402   03-1 $59,928

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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D. S. Chemla - (510) 486-4999/FTS 451-4999

Metallurgy and Ceramics - 01 -

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

107. NATIONAL CENTER FOR ELECTRON MICROSCOPY
U. Dahmen
(510) 486-4627   01-1 $1,720,000

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

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

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

109. ALLOY PHASE STABILITY
D. de Fontaine, L. Falicov
(510) 642-8177 01-1 $226,000

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

110. CAM CERAMIC SCIENCE PROGRAM
Lutgard C. De Jonghe
(510) 486-6138 01-1 $1,302,000

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

111. IN SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY
J. W. Evans
(510) 642-3807 01-1 $50,000

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

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

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

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

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.

114. CAM HIGH PERFORMANCE METALS PROGRAM
J. W. Morris, Jr., R. O. Ritchie, G. Thomas
(510) 486-6482 01-3 $828,000

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

115. SOLID-STATE PHASE TRANSFORMATION MECHANISMS
K. H. Westmacott
(510) 486-5663 01-1 $154,000

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

116. CAM ELECTRONIC MATERIALS PROGRAM
E. Haller, E. Bourret, W. Walukiewicz, J. Washburn, E. Weber
(510) 486-5294 01-3 $909,000

Research in this program focuses on basic material problems pertinent to the development of advanced electronic and optical materials. This includes an integrated semiconductor thin film crystal growth and characterization effort which seeks an understanding of the incorporation of structural and electronic defects, as well as impurities, during the crystal synthesis, post-growth annealing, and/or materials processing. Thrust areas include preparation of single epitaxial layers, formulation of microscopic theories of defect formation in semiconductors, and study of physical and chemical processes affecting incorporation and activation of dopants in II-V compound semiconductors. These studies are complemented by comprehensive investigations of structural properties of heterointerfaces. The objective of this research is to improve understanding of the mechanisms of structural defect formation at heterointerfaces and at surfaces modified by ion beams, and also to reveal a correlation between structural defects and electronic properties of heterointerfaces. A new project has been initiated to study the formation of interfaces between dissimilar materials. Growth by molecular beam, chemical beam and electrochemical epitaxies is combined with in situ and ex situ probes to determine the interplay between growth and properties.

117. HIGH-TEMPERATURE REACTIONS
A. W. Searcy
(510) 486-5900 01-3 $100,000

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

Solid State Physics - 02 -

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

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

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

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

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

The project is a basic science effort with results bearing directly on the technology of plasmas, solid state devices, superconductivity, and magnetic materials.

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

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

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

Development of a new method to determine the in situ structure at metal/solution interfaces using total reflection of X-rays from metal surfaces at glancing incidence and analysis of Bragg reflection parallel and perpendicular to the reflecting plane to obtain complete structural characterization of the interfacial region. Proof-of-principle experiments conducted on the 54-pole wiggler beam line at Stanford Synchrotron Radiation Laboratory (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.

122. FEMTOSECOND DYNAMICS IN CONDENSED MATTER
C. V. Shank
(510) 486-5111 02-2 $190,000

The goal of this research program is to further the basic understanding of ultrafast dynamic processes in condensed matter. Research efforts are focused 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 nm to 800 nm, providing the capability to investigate a large variety of important materials. Recent work has focused on ultrafast scattering events in bulk semiconductors (GaAs), quantum-well semiconductor structures (GaAs/AlGaAs), and semiconductor quantum dots (CdSe microcrystallites). Using laser pulses of only a few optical cycles in duration, we are able to excite highly non-thermal (and non-Fermi) carrier populations. Measurements of the carrier dynamics on a femtosecond time scale provide important insight to fundamental scattering processes in nonequilibrium systems. We have observed the dynamic dephasing of optically created electron-hole pairs. This dephasing occurs due to carrier-carrier scattering. Detailed measurements of this dephasing using photon-echo techniques has enabled us to study the effects of the Coulomb interaction on the scattering events. Such measurements are now being extended to quantum-dot materials in order to further understand the effects of electron confinement as well as surface trapping phenomena. These studies of ultrafast processes in solids will provide new information about the fundamental properties of materials. This knowledge will be useful for evaluating novel materials for energy applications.

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

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

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

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

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

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

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

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

127. CAM HIGH-T_c SUPERCONDUCTIVITY PROGRAM
A. Zettl, P. Berdahl, J. Clarke, R. Gronsky,
N. E. Phillips, A. Portis, P. Richards, E. Weber, P. Yu
(510) 642-4939 02-5 $629,000

Studies in four areas: basic science, thin films and their applications and processing for bulk conductors, and electron microscopy. Basic science (N. E. Phillips) activities are directed at developing an understanding of the known high-T_c materials in the expectation that it will lead to other materials with superior properties. It includes theoretical work, the synthesis of new materials, growth of single crystals, and the measurement of physical properties (including magnetic susceptibility, transport properties, specific heat, mechanical properties, nonlinear electrodynamics, microwave absorption, nuclear magnetic resonance, electron tunneling, and infrared absorption. Theoretical studies include first principles calculations and model-based interpretations of measured properties. Thin films and applications research (J. Clarke) includes fabrication and processing, investigation of physical and electrical properties, development of thin-film devices, including SQUIDS and other applications of Josephson devices, and bolometric radiation sensors. Processing research (L. C. DeJonghe) is directed at understanding and overcoming problems in producing high-current capacity conductors, leading to improved ceramic production of grain-oriented bulk materials and characterization of their electrical and microstructural properties. The electron microscopy research (R. Gronsky) features atomic resolution imaging of cations, which enables defects, grain boundary structure, interface epitaxy, and composition to be analyzed and related to synthesis conditions and to physical properties.

Materials Chemistry - 03 -

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

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128. LOW-TEMPERATURE PROPERTIES OF MATERIALS
N. E. Phillips
(510) 642-6063 03-1 $161,000

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

129. CAM POLYMERS AND COMPOSITES PROGRAM
M. M. Denn, M. D. Alper, M. Bednarski, A. Chakraborty, J. F. Kirsch, D. E. Koshland, P. G. Schultz, C-H. Wong
(510) 642-0176 03-2 $1,004,000

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

130. TWO PERCENT HETEROINTERFACES
J. Kortright, M. Olmstead, J. Porter
(510) 486-5960 03-2 $500,000

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

131. ELECTROCHEMICAL PHASE BOUNDARIES
R. H. Muller
(510) 462-6079 03-2 $120,000

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

132. PHOTOACTIVE POLYMERS FOR PATTERNABLE ORGANIC CONDUCTORS AND SEMICONDUCTORS, PROGRESS TOWARDS THE POLYMERIC CHIP
B. Novak
(510) 643-7536 03-2 $60,000

This project involves the synthesis of normally highly insulating polymeric materials, which when potolyzed, can be converted to fully-conjugated polyacetylene and/or polyacetylene derivatives. Polyacetylene is selected because of its own known high metallic conductivity and its ability to form either p- and n-doped materials. Controlled doping of these photolyzed regions should result in the formation of circuits and device features displaying conductivities ranging from the semiconductor to metallic conductor values and possessing either p- and n-doped charge carries. Specially soluble, insulating, precursor polymers are synthesized and fashioned into thin films. These polymeric films can then be masked to expose only the incipient electrical circuit, and photolyzed. The photolyzed regions are designed to either undergo reaarangements or photofragmentation to produce an insoluble polyacetylene circuit etched into the soluble precursor polymer. At this point, the precursor polymer can be washed away leaving polyacetylene wires and regions (incipient device features) which can then be readily p- or n-doped.

133. ELECTROCHEMICAL PROCESSES
C. W. Tobias
(510) 642-3764 03-2 $60,000

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

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

Experimental data are being obtained for the development of models to predict the behavior of gases, refractory containment materials, and many metallic systems. A thermodynamic data compilation for all elements from H to Lr and their oxides in solid, liquid, and gaseous states from 298 to 3000K 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.

135. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES
D. R. Olander
(510) 642-7055 03-3 $212,000

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.

136. NUCLEAR MAGNETIC RESONANCE
A. Pines
(510) 642-6097 03-3 $740,000

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

137. INTERFACIAL MATERIALS AND PROCESSES
J. D. Porter
(510) 643-7236 03-3 $50,000

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

138. TRIBOLOGY
M. Salmeron
(510) 486-6230 03-3 $250,000

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

139. CAM SURFACE SCIENCE AND CATALYSIS PROGRAM
G. A. Somorjai, A. T. Bell, J. Clarke, S. Louie, M. Salmeron, R. Shen, M. A. Van Hove
(510) 642-4053 03-3 $1,437,000

The Surface Science and Catalysis program emphasizes atomic level surface characterization and the relationship between macroscopic chemical and mechanical properties and properties on the molecular scale. The Surface Science effort includes studies of atomic scale surface structure of solids and adsorbed monolayer; 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. The Surface Instrumentation project develops new surface science techniques including nonlinear optical techniques (sum freqency generation), the scanning tunneling and atomic force microscopies, Raman spectroscopy, and diffuse low energy electron diffraction. 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 bodying modifiers are explored. Catalyzed reactions of interest include selective hydrocarbon conversion to produce clean fuels, nitrogen oxide reduction, hydrogenation and methanol synthesis.

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

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

Facility Operations - 04 -

141. 1-2 GEV SYNCHROTRON LIGHT SOURCE PREOPERATIONS x. 6166
~~J. N. Marx~~ Brian Kincaid
(510) ~~486-5244~~ 486-4810 04-1 $10,481,000 x. 4067
FAX x. 7696

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

LAWRENCE LIVERMORE NATIONAL LABORATORY

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Livermore, CA 94550

T. Sugihara - (510) 423-8351/FTS 543-8351

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

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

143. 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 $520,000

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

144. OPTICAL MATERIALS RESEARCH
L. L. Chase, A. Hamza, H. Lee, S. Payne
(510) 422-6151 02-2 $754,000

Linear and nonlinear optical properties of optical materials are investigated; behavior of surface and bulk properties at high laser intensities is emphasized. Properties measured and modeled include absorption and emission spectra and cross sections, lifetimes of optical excitations, nonlinear transmission and propagation effects, and the effects of intense laser excitation on changes in surface properties, such as desorption, ablation, and optical damage. Coherence properties of optical excitation and ultra-high intensity behavior of materials are investigated with subpicosecond time resolution. Physical and chemical mechanisms for laser-surface interactions on nominally transparent surfaces are investigated using spatially and temporarily resolved photoemission of ions, electrons and neutrals, scanning force microscopy, and surface chemical and structural analysis. 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.

LOS ALAMOS NATIONAL LABORATORY

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R. J. Jensen - (505) 667-1600/FTS 843-1600

Metallurgy and Ceramics - 01 -

D. M. Parkin - (505) 667-9243

145. NEUTRON IRRADIATION INDUCED METASTABLE STRUCTURES
K. E. Sickafus, Jr. Clinard, F. W., M. Nastasi
(505) 665-3457 01-4 $269,000

Irradiation phenomena and damage microstructures resulting from neutron irradiation of ceramics and intermetallic compounds. Investigation of cascae 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.

146. SYNTHESIS AND PROCESSING OF SINGLE CRYSTAL SAPPHIRE FILAMENTS
W. R. Blumenthal
(505) 667-0986 01-5 $235,000

The goal of this project is two-fold and uses a multiple disciplinary approach to study single crystal sapphire filaments for potential use as high temperature creep resistant composite reinforcements. One objective is to empirically relate growth parameters used to control the Edge-defined Film-growth (EGF) and the Laser-heated Floating

Film-growth (EGF) and the Laser-heated Floating Zone processes to resulting microstructures and mechanical properties. A more challenging objective is to model the EFG process in order to not only optimize growth conditions for sapphire, but also for other candidate reinforcement oxides (e.g., YAG). Microstructural and mechanical property characterization meachanisms controlling filament strength.

147. INTERFACIAL AND RADIATION EFFECTS IN STRUCTURAL AND SUPERCONDUCTING CERAMICS
T. E. Mitchell, A. L. Graham, J. J. Petrovic, K. E. Sickafus
(505) 667-0938 01-5 $630,000

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

148. MECHANICAL BEHAVIOR OF VERY HIGH TEMPERATURE STRUCTURAL CERAMICS
T. E. Mitchell, U. F. Kocks, J. J. Petrovic, D. S. Phillips, M. G. Stout
(505) 667-0938 01-5 $265,000

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

149. METASTABLE PHASES AND MICROSTRUCTURES
R. B. Schwarz, T. E. Mitchell
(505) 667-8454 01-5 $255,000

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

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

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes, Bauschinger effects. Characteristics of mechanisms controlling the large strain deformation of aluminum, nickel, iron, copper, brass, 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. Alumina/niobium interface fracture. Measurements of mixed mode fracture energies of homogeneous materials and interfaces between material couples. Fractographic and analytic analysis of interface fracture.

Solid State Physics - 02 -

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

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

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

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

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

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

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

154. HIGH-TEMPERATURE SUPERCONDUCTIVITY
Z. Fisk, A. Arko, P. C. Hammel, I. Raistrick, J. D. Thompson
(505) 667-4476 02-5 $673,000

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

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

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

Materials Chemistry - 03 -

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

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

This is a core program in condensed matter and materials theory aimed at extending the theory base available for modelling novel 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-modeling programs at Los Alamos and elsewhere. The modeling is aimed at both the basic electronic structure of strongly correlated materials, and the development of interatomic potentials for directionally bonded materials.

157. ORIGINATING SUPER-STRONG LIQUID-CRYSTALLINE POLYMERS
F. Dowell, B. C. Benicewicz, R. Liepins
(505) 667-8765 03-2 $524,000

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

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

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

Facility Operations - 04 -

159. LANSCE OPERATIONS SUPPORT, SPECTROMETER DEVELOPMENT, AND USER SUPPORT
R. Pynn
(505) 667-6069 04-1 $5,481,000

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

NATIONAL RENEWABLE ENERGY LABORATORY

1617 Cole Boulevard
Golden, CO 80401

R. A. Stokes - (303) 231-7625/FTS 237-7625

Metallurgy and Ceramics - 01 -

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

160. GROWTH AND PROPERTIES OF NOVEL ORDERED II-VI AND III-V SEMICONDUCTOR ALLOYS
A. Mascarenhas, J. Olson, A. Zunger
(303) 231-1105 01-1 $250,000

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

Solid State Physics - 02 -

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

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

First-principles band structure, total energy, and statistical mechanical (cluster variation and Monte Carlo) methods are used to predict electronic and structural properties of bulk and epitaxial semiconductors superlattices, surfaces and alloys emphasizing chemical trends and properties of new materials. Current work includes (1) first-principles prediction of alloy thermodynamic quantitites (e.g., phase-diagrams) for bulk $A_xB_{1-x}C$ semiconductor alloys including order/disorder transitions, miscibility gaps, and ordered stoichiometric compounds. These methods are also applied to metallic cases, e.g., CuPd, CuAu, CuPt; (2) spontaneous ordering in ternary compounds (e.g., $(GaAs)_m$, $(GaSb)_n$ or HgTe/CdTe superlattices); (3) calculation of valence band offsets between II-VI and III-V semiconductors; (4) prediction of properties of unusual ternary materials, e.g., ordered vacancy $A^{II}B_2^{III}C_4^{IV}$ compounds (e.g., $CdIn_2Se_4$), (5) order-disorder transitions in ternary chalcopyrites (e.g., $CuInSe_2$ and magnetic semiconductors (e.g., MnTe); (6) Surface calculations for semiconductor alloys. 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 simulations of Ising models derived from first-principles.

OAK RIDGE ASSOCIATED UNIVERSITIES

Oak Ridge, TN 37831

A. Wohlpart - 615/576-3255/FTS 626-3255

Metallurgy and Ceramics - 01 -

162. SHARED RESEARCH EQUIPMENT PROGRAM (SHARE)
N. D. Evans, E. A. Kenik
(615) 576-4427 01-1 $128,000

Application of microanalysis facilities for collaborative research in materials science by members of universities or industry with ORNL staff members. Facilities are available for state-of-the-art analytical transmission electron microscopy, atom probe/field ion microscopy, nuclear microanalysis, and mechanical properties measurements at high spatial resolution. Analytical electron microscopy capabilities include energy dispersive X-ray spectroscopy (EDXS), parallel and serial collection electron energy loss spectroscopy (EELS), and convergent beam electron diffraction (CBED). High resolution electron microscopy, high temperature (1500K) or deformation in situ studies, and video recording are available. Surface analysis facilities include three Auger electron spectroscopy (AES) systems and three (0.4, 2.0, and 5.0 MV) Van de Graaff accelerators for Rutherford backscattering and nuclear reaction techniques. A mechanical properties microprobe (Nano-indenter), having high lateral (0.3 μm) and depth (0.16 nm) resolution, can characterize elastic/plastic behavior in thin films, layers, interfaces, and other sub-micron features.

163. OAK RIDGE SYNCHROTRON ORGANIZATION FOR ADVANCED RESEARCH
P. Zschack, R. DeAngelis, S. Moss, C. J. Sparks, Jr., R. Young
(516) 282-5614 01-1 $145,000

A synchrotron radiation beam line installed by the Oak Ridge National Laboratory at the National

Synchrotron Light Source (NSLS) at Brookhaven is made available to interested users from university and industrial laboratories. University staff and industrial scientists are invited to join in collaborative research in materials science of importance to DOE programs at an intense X-ray research facility not available at their home institutions. More than twenty institutions are presently members. The beam line supplies focused X-radiation spanning the energy spectrum from 3 to 40 keV at energy resolutions of delta E/E = 2 x 10^{-4}. One Oak Ridge Associated University staff member is stationed at the NSLS to interface with the users and to assist in their experiments. Research capabilities include crystallography on small samples, structure of amorphous materials both liquid and solid, diffuse X-ray scattering from crystalline defects, short-range order and atomic displacements, interface studies, and X-ray spectroscopy of electron rearrangements. The University of Illinois participates in the operation of this beam line.

OAK RIDGE NATIONAL LABORATORY

P. O. Box 2008
Oak Ridge, TN 37831-6117

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

Metallurgy and Ceramics - 01 -

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

164. MICROSCOPY AND MICROANALYSIS
J. Bentley, E. A. Kenik, M. K. Miller
(615) 574-5067   01-1 $812,000

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

165. X-RAY RESEARCH USING SYNCHROTRON RADIATION
C. J. Sparks, Jr., G. E. Ice, E. D. Specht
(615) 574-6996   01-1 $410,000

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

166. THEORETICAL STUDIES OF METALS AND ALLOYS
G. M. Stocks, W. H. Butler, C. L. Fu, G. S. Painter, N. Wright
(615) 574-5103   01-1 $939,000

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

167. RADIATION EFFECTS
L. K. Mansur, R. A. Buhl, K. Farrell, E. H. Lee, M. B. Lewis, D. Pedraza, R. E. Stoller
(615) 574-4797 01-4 $1,477,000

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

168. TOUGHENING AND RELATED PROCESSING MECHANISMS IN CERAMICS
P. F. Becher, K Alexander, A. Bleier, C.-H. Hsueh
(615) 574-5157 01-5 $986,000

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

169. FUNDAMENTALS OF WELDING AND JOINING
S. A. David, J. M. Vitek, T. Zacharia
(615) 574-4804 01-5 $464,000

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

170. STRUCTURE AND PROPERTIES OF SURFACES AND INTERFACES
L. L. Horton, C. J. McHargue
(615) 574-5081 01-5 $695,000

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

171. HIGH TEMPERATURE ALLOY DESIGN
C. T. Liu, E. P. George, J. A. Horton, W. C. Oliver, J. H. Schneibel, M. H. Yoo
(615) 574-4459 01-5 $1,231,000

Design of ordered intermetallic alloys based on Ni_3Al FeAl and other aluminides (e.g., $TiAl_3$). Study of the effect of alloy stoichiometry on structure and properties of grain boundaries, nature and effects of point defects, and microalloying and grain-boundary segregation. Study of superlattice dislocation structure, solid-solution hardening, mechanistic modeling of anomalous temperature dependence of yield stress, and deformation and fracture behavior of aluminides in controlled environments at 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.

(615) 576-0227

Solid State Physics - 02 9694

Jim Roberto - (615) 574-6151

172. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS
R. M. Moon, J. W. Cable, J. Fernandez-Baca, H. A. Mook, R. M. Nicklow, H. G. Smith
(615) 574-5234 02-1 $940,000

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

173. STRUCTURE AND DYNAMICS OF ENERGY-RELATED MATERIALS
R. M. Moon, H. R. Child, J. B. Hayter, H. A. Mook, S. Spooner, G. D. Wignall
(615) 574-5234 02-1 $1,350,000

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.

174. PROPERTIES OF ADVANCED CERAMICS
J. B. Bates, Y. Chen, N. J. Dudney, G. R. Gruzalski, F. A. Modine, J. R. Noonan, A. L. Wachs
(615) 574-6280 02-2 $543,000

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

175. SYNTHESIS AND PROPERTIES OF NOVEL CERAMIC AND NANOCOMPOSITE AND MACROMOLECULAR THIN FILMS
J. B. Bates, N. J. Dudney, J. R. Noonan, A. L. Wachs
(615) 574-6280 02-2 $495,000

Synthesis of thin films using combinations of physical vapor and chemical vapor deposition techniques such as magnetron and/or ion beam sputtering and plasma polymerization. Types of films include (1) ceramic-ceramic and ceramic-polymer 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.

176. SYNTHESIS AND PROPERTIES OF NOVEL MATERIALS
L. A. Boatner, M. M. Abraham, C. B. Finch, H. E. Harmon, J. O. Ramey, B. C. Sales
(615) 574-5492 02-2 $1,300,000

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

177. PHYSICAL PROPERTIES OF SUPERCONDUCTORS
D. K. Christen, H. R. Kerchner, C. E. Klabunde, J. R. Thompson
(615) 574-6269 02-2 $420,000

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

178. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION
D. H. Lowndes, D. J. Eres, D. B. Geohegan, G. E. Jellison, D. P. Norton
(615) 574-6306 02-2 $880,000

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

179. SMALL ANGLE X-RAY SCATTERING
G. D. Wignall, J. S. Lin, S. Spooner
(615) 574-5237 02-2 $176,000

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.

180. THEORY OF CONDENSED MATTER
J. F. Cooke, J. H. Barrett, H. L. Davis, R. Fishman, K. Flensberg, M. S. Jonon, T. Kaplan, S. H. Liu, G. D. Mahan, G. D. Mostoller, O. S. Oen, S. Pettersson, M. Rasolt, M. T. Robinson, J. C. Wang, R. F. Wood
(615) 574-5787 02-3 $949,000

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

181. STRUCTURAL PROPERTIES OF MATERIALS - X-RAY DIFFRACTION
B. C. Larson, J. D. Budai, M. D. Galloway, J. Z. Tischler
(615) 574-5506 02-4 $462,000

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

182. ELECTRON MICROSCOPY OF MATERIALS
S. Pennycook, M. F. Chisholm, D. Jesson
(615) 574-5504 02-4 $640,000

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

183. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND RESEARCH CENTER
C. W. White, J. L. Moore, O. E. Schow, III, T. P. Sjoreen, D. K. Thomas, S. P. Withrow
(615) 574-6295 02-5 $1,808,000

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.

184. ION BEAM ANALYSIS AND ION IMPLANTATION
C. W. White, M. J. Aziz, J. H. Barrett, M. K. Elghor, R. Feenstra, S. Gorbatkin, J. D. Gresset, O. W. Holland, J. C. McCallum, C. J. McHargue, D. B. Poker, O. E. Schow, J. M. Williams, S. P. Withrow
(615) 574-6295 02-5 $613,000

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 deposited by electron beam evaporation and laser ablation, fundamental studies of ion beam mixing in metal/semiconductor, metal/metal, and metal/insulator systems, applications of ion beam mixing and ion implantation to corrosion/catalysis studies, to reduction of friction and wear of metal surfaces, to changes in mechanical and optical properties of ceramics and insulators, and to reduction of corrosive wear of surgical alloys, formation of epitaxial thin films and layered structures by direct ion beam deposition, studies of ion channeling phenomena.

185. INVESTIGATIONS OF SUPERCONDUCTORS WITH HIGH CRITICAL TEMPERATURES
F. W. Young, Jr., L. A. Boatner, J. Brynstead, B. C. Chakoumakos, D. K. Christen, D. M. Kroeger, S. H. Liu, H. A. Mook, B. C. Sales, S. T. Sekula, J. R. Thompson
(615) 574-5501 02-5 $707,000

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

186. SURFACE PHYSICS AND CATALYSIS
D. M. Zehner, A. F. Baddorf, H. L. Davis, J. R. Noonan, G. W. Ownby, J. F. Wendelken, J. K. Zuo
(615) 574-6291 02-5 $892,000

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

187. ION BEAM DEPOSITION
R. A. Zuhr, T. E. Haynes
(615) 576-6722 02-5 $392,000

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

Materials Chemistry - 03 -

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

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

Application of ion implantation and ion beam mixing to the generation and systematic study of surface-modified materials of interest as catalysts, e.g., $MxTi_{1-x}O_2/Ti$ (M = Ru, Ir, Rh, etc.) for electrocatalysis of Cl_2 and O_2 evolution; determination of the reaction mechanism, the specific catalytic activities, and the electronic properties of the catalysts via electrochemical, Rutherford backscattering, and in situ photoacoustic and photocurrent spectroscopic techniques. Development of new generalized methodologies for the synthesis of nonoxidic ceramic materials (BN, Si_3N_4, SiC, C-B-N ternaries, and borides, carbides, carbonitrides, and nitrides of the transition metals of groups 4, 5, and 6) in powder, fiber, film, or whisker forms; pyrolysis or photolysis of inorganic or organometallic precursors; synthesis of semiconducting C-N-B thin films via pyrolysis of borazine derivatives. Synthesis of TiN whiskers via reactions of titanates with NaCN or NH_3 at high temperatures; topochemically specific solid-state reactions. Synthesis and characterization of high-T_c superconducting oxides; composition/structure/property relationships and their utilization in optimization of synthesis/processing.

189. NUCLEATION, GROWTH, AND TRANSPORT PHENOMENA IN HOMOGENEOUS PRECIPITATION
C. H. Byers, O. A. Basaran, M. T. Harris
(615) 574-4653 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. Investigation of metal alkoxide/metal salt reactions and reactants-solvent interactions (i.e., short-range bonding) which affect the characteristics of the particles formed. Determination of transport properties (i.e., viscosity and diffusivity) which provide important clues to the behavior of the fluid media in which particle growth occurs. Methods and instrument development (including alternative methods for metal oxide powder synthesis, optical spectroscopic measurements, low angle-light scattering spectrometer design, dispersion stabilization, and mathematical analysis).

190. THERMODYNAMICS AND KINETICS OF ENERGY-RELATED MATERIALS
T. B. Lindemer, C. M. Taylor, F. A. Washburn
(615) 574-6850 03-2 $294,000

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

J-2

thermodynamic interrelationship of temperature, oxygen partial pressure, and nonstoichiometry in oxide compounds having extensively variable oxygen-to-metal ratios. Presently, these interrelationships are being measured and modeled for superconducting oxides in the the (Y, lanthanide) barium-copper-oxygen systems. These efforts are providing a heretofore unavailable description of these oxides. The effects of solid-solution carbonate on superconductivity are also being studied.

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

Study of polymeric materials by neutron and X-ray scattering, calorimetry, atomic force microscopy, and statistical mechanical calculations. 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 crystalline, amorphous, and liquid polymers, and the dynamics of materials ranging from oriented fibers to isotropic materials. Development of ways of predicting polymer properties resulting from various processing methods.

Facility Operations - 04

192. ADVANCED NEUTRON SOURCE
C. D. West, R. M. Harrington, J. B. Hayter, B. H. Montgomery, D. L. Selby, P. B. Thompson
(615) 574-0370 04-1 $600,000

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

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

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

Metallurgy and Ceramics - 01 -

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

193. MICROSTRUCTURAL MODIFICATION IN CERAMIC PROCESSING USING INORGANIC POLYMER DISPERSANTS
G. J. Exarhos, W. D. Samuels, I. A. Aksay (U. of Wash)
(509) 375-2440 01-1 $462,000

Fundamental studies of particle compaction phenomena in colloidal processing of ceramics using inorganic polymer dispersants. Localized particle-polymersolvent interactions probed by means of in situ molecular spectroscopic measurements. Integration of spectroscopic data with particle compaction measurements is used to evaluate packing efficiency and relate it to chemical functionality of derivatized inorganic polymer dispersants. Response of bound polymers in the greenbody to high temperatures during sintering also is being investigated. Improvement in mechanical properties of the fired ceramic is correlated with void density and distribution which evolve during processing and with the generation of interfacial phases formed by incorporation of the polymer dispersant with the ceramic matrix.

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

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

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

Development of structure/property relationships for ceramic using systematic variations in bulk and surface/structure, grain size, porosity, and environmental properties. Synthesis of very fine-grained ceramic materials, whose electronic, chemical, and mechanical properties are dominated by their surfaces and grain-boundaries. Develop a fundamental understanding of ceramic surface interactions in a reactive environment through correlations between experimental measurements and molecular modeling. Spectroscopic methods are utilized to investigate initial structures and their evolution in chemically reacting environments. Model systems, electronic structure, and molecular dynamics approaches are emphasized in interpreting molecular-level phenomena. The combination of these techniques is used to extend the molecular information to bulk phenomena.

196. IRRADIATION-ASSISTED STRESS CORROSION CRACKING
S. M. Bruemmer, J. L. Brimhall, E. P. Simonen
(509) 376-0636   01-4 $585,000

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

197. IRRADIATION EFFECTS IN CERAMICS
W. J. Weber, N. J. Hess
(509) 375-2299   01-4 $50,000

Multidisciplinary research on the production, nature, and accumulation of irradiation-induced defects, microsturctures, and solid-state transformations in ceramics. Irradiations with neutrons, ions, and electrons to study point defect production and associate 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/ survivablity, defect stability, and defect migration. The investigations utilize X-ray and neutron diffraction, electron microscopy, EXAFS, laser spectroscopies, ion beam techniques, and electrical property measurements to characterize the defects, microstructures, and transformations introduced by irradiation in simple and complex oxides, carbides, and nitrides. Work includes the development of techniques for in situ characterization during neutron and ion beam irradiations.

Solid State Physics - 02 -

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

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

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

Materials Chemistry - 03 -

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

199. CERAMIC COMPOSITE SYNTHESIS UTILIZING BIOLOGICAL PROCESSES
P. C. Rieke, A. I. Caplan, A. I. Caplan,
B. J. Tarasevich, A. H. Heuer (Case Western)
(509) 375-2833 03-1 $694,000

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

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

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

Metallurgy and Ceramics - 01 -

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

200. PHYSICS AND CHEMISTRY OF CERAMICS
R. A. Assink, C. J. Brinker, B. C. Bunker,
B. D. Kay, J. A. Martin, C.H.F. Pedan,
D. W. Schaefer, J. A. Voigt
(505) 846-2537 01-2 $1,259,000

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

201. ATOMIC LEVEL SCIENCE OF INTERFACIAL ADHESION
T. A. Michalske, B. W. Dodson, J. Hamilton,
J. E. Houston, S. A. Joyce, T. Kitsner, J. Nelson,
P. A. Taylor
(505) 844-5829 01-2 $500,000

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

202. ENERGETIC-PARTICLE SYNTHESIS AND SCIENCE OF MATERIALS
S. T. Picraux, J. C. Barbour, R. J. Bourcier,
B. L. Doyle, M. T. Dugger, D. M. Follstaedt,
J. A. Knapp, S. M. Myers, P. S. Peercy,
P. M. Richards, H. J. Stein, J. Y. Tsao,
W. R. Wampler
(505) 844-7681 01-3 $953,000

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

203. ADVANCED GROWTH TECHNIQUES FOR IMPROVED SEMICONDUCTOR STRUCTURES
S. T. Picraux, P. Bedrossian, D. K. Brice, E. Chason, B. W. Dodson, B. L. Doyle, J. Y. Tsao
(505) 844-7681 01-3 $355,000

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.

204. STRAINED-LAYER SUPERCONDUCTOR MATERIALS SCIENCE
B. W. Dodson, I. J. Fritz, E. D. Jones, J. F. Klem, S. K. Lyo, J. S. Nelson, J. Y. Tsao
(505) 844-6653 01-5 $404,000

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

Solid State Physics - 02 -

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

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

The fundamental physical properties of the oxide-based high temperature superconductors. Directed toward understanding the detailed electronic band structure, doping, and carrier transport in these materials, especially as they pertain to understanding metal-insulator transitions, superconductivity, and the role of oxygen in determining transport properties. 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 0.05K, 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.

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

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

207. VERY HIGH TEMPERATURE SEMICONDUCTING BORIDES
D. Emin, T. L. Aselage, B. Morosin, G. A. Samara, A. C. Switendick, D. R. Tallant, H. L. Tardy
(505) 844-6653 02-5 $516,000

This program investigates boron-rich solids which are refractory materials with uncoventional bondings, structures and properties. The goal is to understand these novel materials and assess their potential for applications. The investigations primarily focus on boron carbides, $B_{12+x}C_{3-x}$, with x between 0 and 1.7, insulating borides including the wide-gap icosahedral boron pnictides, $B_{12}P_2$ and $B_{12}As_2$, and other refractory borides, such as diborides and hexaborides. The materials are synthesized by a variety of techniques. The structural properties, electronic structure, electronic transport (conductivity, Hall effect and Seebeck coefficient measurements) dielectric, optical, magnetic and ultrasonic properties, thermal conductivity and specific heat will be investigated.

Materials Chemistry - 03 -

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

208. CHEMICAL VAPOR DEPOSITION SCIENCES
A. W. Johnson, 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) 844-8782 03-3 $812,000

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

SANDIA NATIONAL LABORATORIES-LIVERMORE

P.O. Box 969
Livermore, CA 94551-0969

P. L. Mattern - (510) 294-2520/FTS 234-2520

Metallurgy and Ceramics - 01 -

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

Phonon and electronic properties of bulk ceramics and the reactivity and structure of ceramic/metal interfaces. Material systems studied include ceramic high temperature superconductors, diamond, and diamond/metal interfaces. Diagnostic techniques utilized are primarily optical and include Raman spectroscopy for the study of phase composition and structure, and infrared spectroscopy, second harmonic generation, and photoemission spectroscopy to study surfaces and buried interfaces. Novel, thin film, ceramic and ceramic metal structures are synthesized using laser ablation deposition. Studies of other advanced ceramics are focused on both the physical and electronic structure of surfaces and interfaces formed with dissimilar materials.

210. GASES IN METALS/COMPUTATIONAL MATERIALS SCIENCE/VISITING SCIENTIST PROGRAM
W. G. Wolfer, D. C. Chrzan, M. S. Daw, T. E. Felter, S. M. Foiles, D. D. Johnson, C. M. Rohlfing, G. J. Thomas, A. F. Wright
(510) 294-2307 01-2 $1,194,000

Investigations of the interactions of hydrogen tritium, helium, and oxygen with metals and metal surfaces and interfaces involving joint theoretical and experimental research. Experimental techniques include high resolution electron microscopy, video low energy electron diffraction, Auger electron spectroscopy, and a Sievert system for charging metal hydrides. New theoretical methods are developed for large-scale atomistic calculations of the structure, properties, and defects in metals and alloys, intermetallic compounds, and semiconductor materials. These methods include the EAM (Embedded Atom Methods), its extension to directionally bonded solids, density functional theory on massively parallel computers, electronic band structure theory for alloys, and quantum chemistry methods for large clusters. These methods are applied to investigate defect clusters in solids, the structure and properties of interfaces, the reconstruction of surfaces, the thermodynamics of alloys, and the bonding and spectroscopic properties of atomic clusters. In addition, stochastic computational methods are developed for modeling the dislocation dynamics in intermetallics, the growth morphology of surfaces and thin films, and the migration of interfaces. A visiting scientist program available to faculty members and students as well as researchers from industry disseminates the computational methods developed.

Solid State Physics - 02 -

211. ADVANCED OPTICAL DIAGNOSTICS FOR INTERFACES AND THIN FILMS
R. H. Stulen, R. J. Anderson, J. C. Hamilton, G. D. Kubiak
(510) 294-2070 02-2 $241,000

Develop, evaluate and apply advanced, nonperturbing diagnostic techniques for studying structure and dynamics of advanced materials. The scope includes studies of bulk, interface and surface properties using coherent, laser-based spectroscopic techniques. Emphasis is on techniques to characterize electronic structure and ultrafast relaxation dynamics using (1) ultrafast laser pulses, extending to the femtosecond regime, (2) one- and two-photon photoemission to study surface electronic structure, and (3) second harmonic generation to study interfaces. Materials under study 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/FTS 462-3153

Facility Operations - 04 -

212. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES
A. I. Bienenstock, H. Winick
(415) 926-3153 04-1 $3,145,000

Support of materials research utilizing synchrotron radiation, as well as operations and development of the Stanford Synchrotron Radiation Laboratory (SSRL). Development and utilization of new methods for determining atomic arrangement in amorphous materials, and on surfaces, time-resolved studies of thin film growth, static and time-resolved studies of highly perfect semiconductor crystals using X-ray topography, photoemission studies of semiconductor interfaces (e.g., heterojunctions and Schottky barriers), metal surfaces (especially catalytic reactions on surfaces) and development of techniques such as surface EXAFS, photoelectron diffraction, photon stimulated desorption and interface studies using core level spectroscopy. Performance and photoelectron spectroscopic studies of catalysts. Development of accelerators and insertion devices for synchrotron radiation production, and development and Lau diffraction for time-resolved protein crystallography. Development of ultra-high resolution scattering techniques, by means of resonant nuclear scattering.

SECTION B

Grant Research

(Primarily Universities)

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

UNIVERSITY OF ALABAMA
Birmingham, AL 35294

213. MIGRATION OF CONSTITUTIONALLY LIQUATED FILMS (CLFM)
R. G. Thompson, Department of Materials Engineering
(205) 934-8450

B. Radhakrishnan, Department of Materials Sciences and Engineering
(205) 934-8450 01-5 $100,000 (16 months)

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

214. STRUCTURE, STOICHIOMETRY AND STABILITY IN MAGNETOPLUMBITE AND B-ALUMINA TYPE CERAMICS
A. N. Cormack, Department of Ceramic Science and Engineering
(607) 871-2180 01-1 $49,042

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

215. MOBILE IONS IN FAST ION CONDUCTING SYSTEMS
C. A. Angell, Department of Chemistry
(602) 965-7217 01-1 $79,373

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

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

S. H. Lin, Department of Chemistry
(602) 965-3715 01-1 $108,600

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.

217. SURFACE STRUCTURES AND REACTIONS OF CERAMICS AND METALS
J. M. Cowley, Department of Physics
(602) 965-6459 02-2 $110,000

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

UNIVERSITY OF ARIZONA
Tucson, AZ 85721

218. ARTIFICIALLY STRUCTURED MAGNETIC MATERIALS
C. M. Falco, Department of Physics
(602) 621-6771 02-2 $100,000

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

BOEING COMPANY
P.O. Box 3999
Seattle, WA 98124

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

F. W. Lytle, Department of Physics
(206) 544-5348 01-1 $69,188

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

BOSTON UNIVERSITY
500 Commonwealth Avenue
Boston, MA 02215

220. THE HEAVY ELECTRON STATE
A. Auerbach, Department of Physics
(617) 353-5787 02-3 $38,310

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 using a time dependent functional integral methodology.

221. STRUCTURE AND DYNAMICAL TRENDS IN 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 $112,400

Use of scattered spin-polarized metastable $He(2^3S)$ atoms from surfaces both elastically and inelastically, to study the structural, dynamic and magnetic trends of the 3D transition metal overlayers-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 (SPMH) facility. The surface magnetic structure of antiferromagnetic transition metal oxides (example, M_nO) will be studied. Computer modeling, employing Friedel oscillations and Double-sine-Gordon surface dislocations, will be used to interpret measured phonon dispersion data.

BROWN UNIVERSITY
Providence, RI 02912

222. FATIGUE CRACK GROWTH UNDER FAR-FIELD CYCLIC COMPRESSION
S. Suresh, Division of Engineering
(401) 863-2626 01-2 $93,405

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

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

J. Tauc, Division of Engineering
(401) 863-2318 02-2 $160,000

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

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

A. K. Mukherjee, Department of Mechanical Engineering
(916) 752-1776 01-2 $128,000

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.

225. INVESTIGATION OF RADIATION DAMAGE AND DECOMPOSITION OF CERAMICS USING ELECTRON MICROSCOPY
D. G. Howitt, Department of Mechanical Engineering
(916) 752-0580 01-4 $95,000

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

UNIVERSITY OF CALIFORNIA AT IRVINE
Irvine, CA 92717

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

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

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

227. OPTICAL STUDIES OF MOLECULAR ADSORBATES
J. C. Hemminger, Department of Chemistry
(714) 856-6020 02-2 $157,000

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

228. INELASTIC ELECTRON SCATTERING FROM SURFACES
D. L. Mills, Department of Physics
(714) 856-5148 02-3 $130,000

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 spin-flip scattering of low energy electrons from magnetic excitations at surfaces, and excitation of surface phonons by helium atoms. Strong emphasis on the quantitative comparison between the results of this program and experimental data. Tightly coupled effort between Professor Mills and Professor Tong at the University of Wisconsin at Milwaukee.

UNIVERSITY OF CALIFORNIA AT LOS ANGELES
Los Angeles, CA 90024

229. IRRADIATION-INDUCED DISORDERING, DUCTILITY AND PHASE TRANSFORMATIONS IN ORDERED INTERMETALLIC COMPOUNDS
A. J. Ardell, Department of Materials Science and Engineering
(213) 825-7011 01-4 $84,599

Proton irradiation of ordered intermetallic compounds at temperatures from -175 C to room temperature. Investigation of irradiation-induced ductility in L_{12} and B_2 compounds. Irradiated specimens mechanically tested in bending, and fracture surfaces studied for assessment of ductility. Specimen examination by TEM, X-ray diffraction, and electron diffraction. Identification and characterization of tweed-like reaction product of a phase transformation in proton-irradiated hypostoichiometric Ni_3Al.

230. APPLICATION 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 $54,730 (9 months)

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

231. SUPERCONDUCTIVITY AND MAGNETISM IN D- AND F-ELECTRON MATERIALS
M. B. Maple, Department of Physics
(619) 534-3330 02-2 $375,000

Investigations on a variety of rare-earth and actinide compounds, including studies of superconductivity, magnetism, and effects that arise from their mutual interaction, as well as the anomalous behavior exhibited by heavy electron (heavy Fermion) materials that is associated with valence fluctuations and the Kondo effect. Measurements of ac and dc magnetic susceptibility, specific heat, and electrical resistivity under conditions of temperature between 80 millikelvin and 300K, magnetic fields to 10 Tesla, and pressures to 160 kilobar. Search for new high-T_c superconducting materials and characterization of their properties, including 4f electron hybridization effects, magnetic ordering, growth of single crystals and measurement of upper critical fields and critical current densities.

232. PREPARATION AND CHARACTERIZATION OF SUPERLATTICES
I. K. Schuller, Department of Physics
(619) 534-2540 02-2 $105,000 (7 months)

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

233. ION MIXING OF SEMICONDUCTOR LAYERED-STRUCTURES
S. S. Lau, Department of Electrical Engineering and Computer Sciences
(619) 534-3097 02-4 $135,000

Experimental investigation of layer disordering by ion mixing in semiconductor quantum-well and superlattice structures. Emphasis on determining the disordering mechanisms of semiconductor layered-structures under ion bombardment. Issues 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. Goal is to develop a unified mechanism for ion mixing in such materials.

UNIVERSITY OF CALIFORNIA AT SANTA BARBARA
Santa Barbara, CA 93106

234. FUNDAMENTAL STUDIES OF THE INTERRELATIONSHIP BETWEEN GRAIN-BOUNDARY PROPERTIES AND THE MACROSCOPIC PROPERTIES OF POLYCRYSTALLINE MATERIALS
D. R. Clarke, Materials Department
(805) 893-8232 01-1 $100,000

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. Comparison of results from polycrystalline thin films and composed to simulations.

235. STRUCTURE AND CHEMISTRY OF METAL/CERAMIC INTERFACES
A. G. Evans, Materials Department
(805) 961-8275 01-1 $52,746 (24 months)

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

236. THEORIES OF PATTERN FORMATION AND NONEQUILIBRIUM PROCESSES
J. S. Langer, Department of Physics
(805) 963-4111 02-3 $135,000

Theoretical investigation 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.

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

J. R. Schrieffer, Department of Physics
(805) 893-2800 02-3 $90,000 (9 months)

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

238. MOLECULAR PROPERTIES OF THIN ORGANIC INTERFACIAL FILMS
J. Israelachvili, Department of Chemical and Nuclear Engineering
(805) 961-3412 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 0.1 nm. Adhesion and surface energy of metals coated with surfactant and polymer films are measured by SFA in both gaseous and liquid environments. New measurements of dynamic forces acting on two laterally moving surfaces, recording the normal (compressive) and tangential (frictional) forces while simultaneously monitoring the plastic deformation.

239. INTERFACIAL PROPERTIES OF CHARGED MACROMOLECULES
P. A. Pincus, College of Engineering-Engineering Materials Program
(805) 893-4685 03-2 $98,600

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

240. PHASE TRANSITIONS IN SYSTEMS WITH QUENCHED DISORDER
D. Belanger, Department of Physics
(408) 459-2871 02-1 $60,000 (9 months)

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

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA 91125

241. ORDERING PHENOMENA IN UNDERCOOLED ALLOYS
B. T. Fultz, Department of Engineering
(818) 356-2170 01-1 $83,810

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

242. STUDIES OF ALLOY STRUCTURES AND PROPERTIES
W. L. Johnson, Division of Engineering and Applied Science
(818) 356-4433 01-1 $238,922

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

243. GRAIN-BOUNDARY AND INTERFACE KINETICS DURING ION IRRADIATION
H. A. Atwater, Department of Applied Physics
(818) 356-2197 01-4 $91,398

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

244. MELTING IN ADSORBED FILMS
D. L. Goodstein, Department of Physics, Mathematics, and Astronomy
(818) 356-4319 02-2 $90,000

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

CARNEGIE MELLON UNIVERSITY
3325 Science Hall
Pittsburgh, PA 15213

245. THE EFFECTS OF APPLIED STRESS ON MICROSTRUCTURAL EVOLUTION
W. C. Johnson, Department of Metallurgical Engineering and Materials Science
(412) 268-8785 01-1 $98,600

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

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

D. N. Lambeth, Department of Electrical and Computer Engineering
(412) 268-3674 01-1 $95,000

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. Interelationship of microstructure, magnetic domain structure and extrinsic magnetic properties of magnetic thin films.

247. PHASE SEPARATION AND ORDERING IN INGaAsP AND INGaAs MATERIALS
S. Mahajan, Department of Metallurgical Engineering and Materials Sciences
(412) 268-2702

D. E. Laughlin, Department of Metallurgical Engineering and Materials Sciences
(412) 268-2706 01-1 $130,000 (18 months)

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

248. INVESTIGATION OF THE INTERPLAY BETWEEN COMPOSITION AND STRUCTURE AT INTERPHASE BOUNDARIES
P. Wynblatt, Department of Metallurgical Engineering and Materials Science
(412) 268-8711 01-1 $103,530

Combined experimental and theoretical study of the relation between composition and structure of solid/solid interphase boundaries. Experimental work to be carried out by: 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. Modeling of interphase boundary structure and composition by Monte Carlo techniques.

249. 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 $98,500

Theoretical study of 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. Understanding of 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.

UNIVERSITY OF CHICAGO
5640 Ellis Avenue
Chicago, IL 60637

250. HIGH-TEMPERATURE THERMOCHEMISTRY OF TRANSITION METAL BORIDES AND SILICIDES
O. J. Kleppa, The James Franck Institute
(312) 702-7198 01-3 $79,159

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. Establishment of systematic trends in the enthalpy of formation for transition metal silicides and borides.

UNIVERSITY OF CINCINNATI
Cincinnati, OH 45221

251. ROLE OF INTERFACIAL PROPERTIES ON THE STEADY STATE AND NON-STEADY STATE FIRST-MATRIX CRACKING BEHAVIORS IN CERAMIC-MATRIX COMPOSITES
R. N. Singh, Department of Materials Science and Engineering
(513) 556-3119 01-5 $80,000

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

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

252. DYNAMICS AND PATTERN SELECTION AT THE CRYSTAL-MELT INTERFACE
H. Z. Cummins, Department of Physics
(212) 690-6921 02-2 $135,000

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

253. MAGNETIC CRITICAL BEHAVIOR OF CONDUCTIVITY NEAR THE M-I TRANSITION
M. P. Sarachik, Department of Physics
(212) 690-6904 02-2 $107,285

A precise systematic study of the magnetic properties of homogeneous, well- characterized samples of heavily doped semiconductors as a function of impurity concentration across the metal-nonmetal transition. Faraday balance measurements as a function of temperature (1.25 to 300K) and of magnetic field (to 50kG) to separate various contributions to the total susceptibility. The measurements will be extended to 500 mK and 190 kG at the National Magnet Laboratory. The role percolation has in the transition will be determined.

254. TRANSPORT IN SMALL AND/OR RANDOM SYSTEMS
M. Lax, Department of Physics
(212) 690-6864 02-3 $115,000

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

255. OPTIMIZATION OF FILM SYNTHESIZED RARE EARTH TRANSITION METAL PERMANENT MAGNET SYSTEMS
F. J. Cadieu, Department of Physics
(718) 997-7463 01-1 $138,040

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

CLARK ATLANTA UNIVERSITY
Atlanta, GA 30314-4381

256. 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 $66,786

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

COLORADO SCHOOL OF MINES
Golden, CO 80401

257. NOVEL CONCEPTS IN WELDING: 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 $120,000

Composite modeling techniques, 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. 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 simulating the composition and microstructure gradients in solidified weld metal. Appropriate mathematical models to evaluate the properties of the composite weld metals.

258. POTENTIAL MODULATION OF EQUILIBRIUM AND EXCITATION PHENOMENA AT THE ELECTROLYTE-SOLID INTERFACE
T. Furtak, Department of Physics
(303) 273-3843   02-2 $100,000

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. Emphasis 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

259. PROPERTIES OF MOLECULAR SOLIDS AND FLUIDS AT HIGH PRESSURE AND TEMPERATURE
R. D. Etters, Department of Physics
(303) 491-6206   02-3 $70,000

Calculation of the properties of molecular solids and fluids over broad ranges of temperature and pressure. Properties of interest. Solids: equilibrium structures and orientations, lattice vibrational and vibrational mode frequencies, intramolecular vibron frequencies, sound velocities, equations of state, compressibilities, 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 and correlation with experimental programs at Los Almos National Laboratory and Lawrence Livermore National Laboratory.

COLUMBIA UNIVERSITY
New York, NY 10027

260. PROTONS AND LATTICE DEFECTS IN PEROVSKITE-RELATED OXIDES
A. S. Nowick, Krumb School of Mines
(212) 854-2921 01-3 $133,000

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

UNIVERSITY OF CONNECTICUT
Storrs, CT 06268

261. A COHERENT MODEL OF MARTENSITIC NUCLEATION AND GROWTH
P. C. Clapp, Department of Metallurgy
(203) 486-4714 01-1 $148,110

Development of coherent martensitic nucleation model for a variety of transformation symmetries using a nonlinear, nonlocal strain free energy similar to the Ginzburg-Landau form. Fourth order gradient terms are included to deal with the large number of real systems showing negative second order strain gradient coefficients; heterogeneous defects of varying potencies are included; the dynamics of the transformation instabilities are analyzed for specific cases. One-, two-, and three-dimensional cases are studied and matched with the parameters of real systems. Point, line, and surface defects are considered and their effects, both local and global, on the transformation are examined. The model contains a self-consistency check on the coherency hypothesis; cases that fail this test are considered separately indicating an essential essential role for interface dislocations in the nucleation process. Comparisons to experimental data on Na, β-NiAl, Fe-30Ni and Nb_3Sn.

262. 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) 486-4924 02-2 $22,825 (3 months)

Local environment changes in electron- and hole-doped systems based on the La_2CuO_4 and the Nd_2CuO_4 systems by varying oxygen activity and ion valences. Careful studies with X-ray near edge (XANES) and extended absorption fine structure spectroscopy (EXAFS) at the National Synchrotron Light Source provide electronic and structural information. Glancing angle X-ray reflectivity and EXAFS of superconducting substrate interactions, transition metal aluminides and implanted transition metal silicide systems will be explored.

263. ENERGY TRANSFER AND NONLINEAR OPTICAL PROPERTIES AT NEAR ULTRAVIOLET WAVELENGTHS: RARE EARTH 4F TO 5D TRANSITIONS IN CRYSTALS AND GLASSES
D. S. Hamilton, Department of Physics
(203) 486-4914 02-2 $21,000

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

CORNELL UNIVERSITY
Ithaca, NY 14853

264. CRYSTALLINE-AMORPHOUS OXIDE INTERFACES AND RELATION TO GRAIN-BOUNDARY FILMS
C. B. Carter, Department of Materials Science and Engineering
(607) 255-4797 01-1 $137,751

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

265. THEORY OF NONLINEAR, DISTORTIVE PHENOMENA IN SOLIDS: MARTENSITIC, CRACK AND MULTISCALE STRUCTURES-PHENOMENOLOGY AND PHYSICS
J. A. Krumhansl, Department of Physics
(413) 253-2704

J. P. Sethna, Department of Physics
(607) 255-5132 01-1 $157,760

Development of a 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. Search for giant elastic softening, glassy properties, nucleation and nucleation dynamics.

266. STUDIES OF THE III-V COMPOUNDS IN THE MEGABAR REGIME
A. L. Ruoff, Department of Materials Science and Engineering
(607) 255-4161 01-1 $129,166

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

267. EXPERIMENTAL STUDIES OF THE STRUCTURE OF GRAIN-BOUNDARIES
S. L. Sass, Deparment of Materials Science and Engineering
(607) 255-5239 01-1 $197,620

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

268. UHV-STEM STUDIES OF NUCLEATION AND GROWTH OF THIN METAL AND SILICIDE FILMS ON SILICON
J. Silcox, School of Applied and Engineering Physics
(607) 255-3332

E. J. Kirkland, School of Applied and Engineering Physics
(607) 255-3332 01-1 $149,166

Compound formation between silicon and heavy transition elements and grain-boundaries in Ni_3Al studied by annular dark field scanning transmission electron microscopy (ADF-STEM) at atomic structure resolution level and by analytical EM. Initial stages of epitaxial elemental or silicide thin film formation in early cluster formation (islands) surface domain and interface formation on silicon. Effects of annealing and contaminant gases (e.g., 0_2, H_2) on observed structures. Structure, chemical composition and local electronic structure of grain-boundaries in Ni_3 determined with annular dark field Z-contrast, convergent beam electron diffraction and EELS.

269. CERAMIC FILMS AND INTERFACES: CHEMICAL AND MECHANICAL PROPERTIES
Rishi Raj, Department of Materials Science and Engineering
(607) 255-4040 01-2 $176,630

Structure and composition of interfaces between dissimilar ceramics and 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.

270. STRUCTURE AND ELECTRONIC PROPERTIES OF MISMATCHED III-V INTERFACES
D. Ast, Department of Materials Science and Engineering
(607) 255-4140 01-3 $92,684

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

271. SURFACE PHASES AND THEIR INFLUENCE ON METAL-OXIDE INTERFACES
J. M. Blakely, Department of Materials Sciences and Engineering
(607) 255-5149 01-3 $112,762

Determination of phase diagrams for binary 2-D adsorbed systems, such as S + O, on transition metal surfaces 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 surface phase morphology, interphase boundaries, and heterogeneous oxide-adsorbate surfaces.

272. DEFECTS AND TRANSPORT IN MIXED OXIDES
R. Dieckmann, Department of Materials Science and Engineering
(607) 255-4315 01-3 $111,500

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.

273. THE GEOMETRY OF DISORDER: QUASICRYSTALS AND FRUSTRATED MAGNETS
C. L. Henley, Department of Physics
(607) 255-5056 02-3 $76,000

Investigate quasicrystal geometry to compute phason elastic constants, compare 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 search for new experimental tests of "spin-density wave," and "Fermi-liquid" models. In percolation and nonlinear dynamics, analytically determine exponents of self-organized percolation model in one dimension and in mean field theory.

274. SYNTHESIS AND PROPERTIES OF NOVEL CLUSTER PHASES
F. J. DiSalvo, Department of Chemistry
(607) 255-7238 03-1 $169,000

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 bi-functional ligands or 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

275. THE HALL-PETCH RELATIONSHIP AND MECHANISMS OF FRACTURE IN B_2 COMPOUNDS
I. Baker, Thayer School of Engineering
(603) 646-2184 01-2 $113,672

An investigation of the relationship between the parameter K, in the Hall-Petch Relationship, $\sigma_y = \sigma_o + Kd^{-1/2}$, 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.

276. INTERGRANULAR FRACTURE AND THE ACCOMMODATION OF SLIP AT GRAIN-BOUNDARIES
E. M. Schulson, Thayer School of Engineering
(603) 646-2888 01-2 $129,229

Examine dislocation pileup/grain-boundary accommodation model in more detail, carry out systematic in situ TEM deformation studies on Ni-rich, stoichiometric and Ni-lean Ni_3Al both with (0.35 at%) and without boron; investigate grain boundary sliding in Ni_3Al by systematic experiments on the effects of grain size on high temperature deformation (800-1200K) of Ni_3Al with (0.35 at%) and without boron; investigate grain size effects on the strength and ductility of Ni_3Si, Ni_3Ge, and Ni_3Ga by systematic experiments on the effects of grain size on the mechanical properties and resultant deformation structure; improve the toughness of intermetallic compounds through grain shape control, i.e., generate equiaxed fine grain structure with simultaneous increase of aspect ratio, comparative tests (fibrous vs equiaxed microstructures) performed at RT using Charpy impact technique. Subsequent fracture toughness measurements using standard ASTM procedures.

277. EXCITONS IN SEMICONDUCTING SUPERLATTICES, QUANTUM WELLS, AND TERNARY ALLOYS
M. D. Sturge, Department of Physics
(603) 646-2359 02-2 $100,929

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 in electron-hole plasmas 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 be examined.

UNIVERSITY OF DELAWARE
Newark, DE 19716

278. FUNDAMENTAL STUDIES OF STRONGLY MAGNETIC RARE EARTH-TRANSITION METAL ALLOYS
G. C. Hadjipanayis, Department of Physics
(302) ~~451~~ 831-2736 02-2 $39,994

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

UNIVERSITY OF DENVER
Denver, CO 80208

279. RESIDUAL STRESSES IN FIBER-REINFORCED CERAMIC COMPOSITES BY DIFFRACTION METHODS
P. K. Predecki, Department of Engineering
(303) 871-3570 01-2 $59,160

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

FLORIDA ATLANTIC UNIVERSITY
Boca Raton, FL 33431

280. THEORETICAL STUDIES OF METALLIC ALLOYS
J. S. Faulkner, Department of Physics
(407) 367-3429

L. T. Wille, Department of Physics
(407) 367-3429 01-1 $69,020

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 and the energies of the ordered phases will be obtained with the QKKR. The subprograms will be integrated using a QKKR-CPA and advanced coding for a supercomputer such as bit mapping and logical operations that will lead to a vectorized code. Realistic first principles calculations of phase diagrams and phase stability parameters will then be performed on the alloys such as PdRh, MoCr, MoNb, MoTa, and other topical systems.

FLORIDA STATE UNIVERSITY
Tallahassee, FL 32306

281. HEAVY FERMIONS AND OTHER HIGHLY CORRELATED ELECTRON SYSTEMS
P. U. Schlottmann, Department of Physics
(904) 644-2246 02-3 $91,296

Theoretical investigations 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.

282. 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 $135,000

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

UNIVERSITY OF FLORIDA
Gainesville, FL 32611

283. QUANTUM-CONFINEMENT EFFECTS AND OPTICAL BEHAVIOR OF INTERMEDIATE SIZE SEMICONDUCTOR CLUSTERS
J. H. Simmons, Department of Materials Science and Engineering
(904) 462-5469

P. H. Kumar, Department of Physics
(904) 392-6690 01-1 $175,067 (16 months)

Relationship between semiconductor microstructure, electronic band structure, and linear and nonlinear optic properties of semiconductor cluster/glass composites; nonvanishing 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 subpicosecond spectral hole burning.

284. THE COUPLING OF THERMOCHEMISTRY AND PHASE DIAGRAMS FOR GROUP III-V SEMICONDUCTOR SYSTEMS
T. J. Anderson, Department of Chemical Engineering
(904) 392-2591 01-3 $88,740

Component activities measured in the compound semiconductor system Ga-In-As-P with solid state electrochemical methods. Ga or In activities measured in liquid solutions with a galvanic cell using yttria-stabilized zirconia as the solid electrolyte. Activity of GaAs in the solid solution $Ga_x3In_{1-x}As$ measured with a galvanic cell. GaAs solidus measured by coulometric titration in an electrochemical cell using MOCVD deposited GaAs. Reference state for Group III arsenides and phosphides will be studied. Infinitely dilute solutions of As or P in In and Ga will be investigated as suitable reference states. Measurement results and reference state characterization studies used to assess the thermochemistry and phase diagram of the Ga-In-As-P system. Results of this assessment will be used for complex chemical equilibrium calculations as applied to hydride CVD in $In_xGa_{1-x}As_yP_{1-y}$. Assessment of Ga-As-Bi and Al-Ga-In-P systems will be performed.

285. X-RAY SCATTERING STUDIES OF NONEQUILIBRIUM ORDERING PROCESSES
S. E. Nagler, Department of Physics
(904) 392-8842 02-2 $65,000

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

286. STUDIES OF NOVEL SUPERCONDUCTORS
G. R. Stewart, Department of Physics
(904) 392-9263 02-2 $100,000

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

GEORGIA TECH RESEARCH CORPORATION
Atlanta, GA 30332

287. 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 $50,000

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.

288. STRUCTURE AND DYNAMICS OF MATERIAL SURFACES, INTERPHASE-INTERFACES AND FINITE AGGREGATES
U. Landman, School of Physics
(404) 894-3368 02-3 $229,266

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

289. GROWTH, STRUCTURE AND STABILITY OF EPITAXIAL OVERLAYERS
A. Zangwill, Department of Physics
(404) 894-7333 02-3 $85,000

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.

290. THE ORGANIC CHEMISTRY OF CONDUCTING POLYMERS
L. M. Tolbert, Department of Chemistry
(404) 894-4043 03-1 $93,670

The phenomena of charge transport in conducting polymers, materials which are ordinarily insulators, is basically a problem in mechanistic organic chemistry. Fundamental studies are being conducted in which 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

291. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS
W. M. Yen, Department of Physics and Astronomy
(404) 542-2491 02-2 $125,000

Investigation of relaxation and energy transfer in and among optically excited states in disordered or amorphous systems and in certain ceramics. Application of new spectroscopic techniques to provide more fundamental understanding of prototypical transport processes. Application of advanced laser techniques, including fluorescence line narrowing (FLN) and time-resolved FLN, Dilution Narrowed Laser Spectroscopy (DNLS), measurement of coherent optical transients, photoacoustic and photocaloric methods, and far infrared free electron laser. Examination of activated materials with proven fractal dimensions and properties, energy transfer across order-disorder environment.

HARVARD UNIVERSITY
Cambridge, MA 02138

292. MEASUREMENTS OF CRYSTAL GROWTH KINETICS AT EXTREME DEVIATIONS FROM EQUILIBRIUM
M. J. Aziz, Division of Applied Science
(617) 495-9884 01-1 $90,000

Time-resolved measurements of optical reflectance, translent 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.

293. X-RAY STANDING WAVE INTERFEROMETRY-OPTICS AT 1 ANGSTROM WITH APPLICATIONS TO SURFACE AND MATERIAL SCIENCES
J. A. Golovchenko, Department of Physics
(617) 495-3905 02-2 $175,000

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

294. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS
I. F. Silvera, Department of Physics
(617) 495-9075 02-2 $210,000

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 microwave traps and cooling and by using helium walls covered with electrons. Attempt to observe directly the surface atoms of spin-polarized hydrogen adsorbed on a helium film surface. Observe the onset of the expected superfluidity in the two-dimensional system by means of "third sound" resonance. Develop a matter wave interferometer.

295. SYNCHROTRON STUDIES OF X-RAY REFLECTIVITY FROM SURFACES
P. S. Pershan, Department of Physics and Applied Science
(617) 495-3214 03-3 $80,495

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

296. DIFFRACTION STUDIES OF THE STRUCTURES OF GLASSES AND LIQUIDS
S. C. Moss, Department of Physics
(713) 749-2840 02-1 $132,000

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

IBM
650 Harry Road
San Jose, CA 95120-6099

297. SEGMENTAL I... ERPENETRATION AT POLYMER-POLYMER INTERFACES
T. P. Russell, Almaden Research Center
(408) 927-1638 03-2 $77,777 (9 months)

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 homopolymers. 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 47402

298. HIGH-RESOLUTION ELECTRON ENERGY LOSS STUDIES OF SURFACE VIBRATIONS
L. Kesmodel, Department of Physics
(812) 855-0776 02-2 $115,902

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
Baltimore, MD 21218

299. INVESTIGATION OF THE PROCESSES CONTROLLING THE FLAME GENERATION OF REFRACTORY MATERIALS
J. L. Katz, Department of Chemical Engineering
(301) 338-8484 01-3 $73,950

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.

300. DE-ALLOYING AND TRANSCRYSTALLINE STRESS-CORROSION CRACKING
K. Sieradzki, Department of Materials Science and Engineering
(301) 338-5409

J. W. Wagner, Department of Materials Science and Engineering
(301) 338-5409 01-5 $80,000

Research addresses three major areas: 1) the dynamics of the film-induced micro-cleavage process; 2) the effect of the electrochemical potential on the coarsening of de-alloyed sponges and 3) the mechanical properties of de-alloyed layers. Test parameters include de-alloyed film thickness foil texture, electrochemical potential, dynamic displacement rates and amplitude of the displacement pulse applied. Examine role of the penetrate into ductile substrate. Measure the propagation of brittle elastic cracks in a 10 micron thick foil coarsening of de-alloyed layers by: 1) electrochemical techniques, 2) grazing angle X-ray scattering and X-ray reflectivity measurements at National Synchrotron Light Source and 3) scanning tunneling microscopy. Mechanical properties of de-alloyed structures to determine the effect of coarsening on the elastic and fracture properties of the layers. Alloy systems include Zn-Cu, Ag-Au and Cu-Au.

LEHIGH UNIVERSITY
Bethlehem, PA 18015

301. ANALYTICAL ELECTRON MICROSCOPY OF CATALYSTS
C. E. Lyman, Department of Metallurgy and Materials Engineering
(215) 861-4249 01-1 $84,844

Elucidation of the processes or phenomena which control the internal distribution of deposited metal during the preparation of supported metal catalysts. Measurement of the distribution of noble and metallic catalytic poisons on a micrometer to nanometer scale by electron beam microanalytical methods. Correlation of catalyst microstructure with catalytic activity. Variable experimental parameters include noble metal type, impregnation procedure, drying rate, reduction rate, type of SO_2 sorbent coating, regeneration scheme, etc. Detailed study of effects of electron beam damage on surface mobility of catalytic poisons. Principle analytical techniques are analytical electron microscopy with a field emission gun and a lateral spatial resolution better than 2 nm and electron probe elemental microanalysis with a spatial resolution of 1 to 10 nm.

302. HIGH RESOLUTION MICROSTRUCTURAL AND MICROCHEMICAL ANALYSIS OF ZIRCONIA EUTECTIC INTERFACES
M. R. Notis, Department of Metallurgy and Materials Sciences
(215) 758-4225 01-1 $116,535

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.

303. THE EFFECT OF POINT DEFECTS AND DISORDER ON STRUCTURAL PHASE TRANSITION
J. Toulouse, Department of Physics
(215) 758-3960 01-1 $81,160

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

304. 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 $128,525

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.

305. ROLE OF STRUCTURE ON ION MOVEMENT IN GLASSES
H. Jain, Department of Materials Science and Engineering
(215) 758-4217 01-3 $60,000

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.

UNIVERSITY OF MAINE
Orono, ME 04469

306. STRUCTURE, ADHESION, AND STABILITY OF METAL/OXIDE AND OXIDE/OXIDE INTERFACES
R. J. Lad, Department of Physics
(207) 581-2257 01-1 $77,000

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

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, MA 02139

307. 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 $517,000

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.

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

P. C. Searson, Department of Materials Science and Engineering
(617) 253-4697 01-1 $73,950

The research is composed of two parts:
(1) 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 (2) identification of the sites of electrochemical processes occurring on electrodes by modeling 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.

309. SLIP, TWINNING AND TRANSFORMATIONS 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) 253-6939 01-2 $176,000 (21 months)

Study effect of alloying, temperature, strain rate, and volume fraction of bcc phase on mechanical twinning and low-temperature deformability in HfV_2-based systems, $TiCr_2$ and Ti-$TiCr_2$ systems, $Mg(Cu,Zn)_2$

and (Zr, Ti)Fe_2 near C15-C14 transitions. Also Mg$(Cu,Zn)_2$ - Cu will be included. Fundamental considerations of synchro-shear processes in slip, twinning, and phase transformations in Laves phases, with goal of determining factors controlling strength, toughness and ductibility in intermetallics.

310. GRAIN-BOUNDARIES IN MULTICOMPONENT CERAMICS
Y. -M. Chiang, Department of Materials Science and Engineering
(617) 253-6471 01-2 $108,459

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

311. OXIDES AND SURFACE MAGNETISM
R. C. O'Handley, Department of Materials Science and Engineering
(617) 253-6913

M. Oliverio, Department of Materials Science and Engineering
(617) 258-6113 01-3 $174,000 (16 months)

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.

312. 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 $123,600

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

313. MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS
J. B. Vander Sande, Department of Materials Science and Engineering
(617) 253-6933 01-3 $186,934

Processing of superconducting oxide/Ag microcomposites by oxidation of metallic precursor alloys including microstructural characterization and electrical property measurements of product phases generated, with emphasis on $YbBa_2Cu_3O_x$/Ag and $(Bi,Pb)_2Sr_2Ca_2Cu_3Oy$/Ag. In addition to specific work on the formation, structure, and properties of superconducting oxide/Ag microcomposites, research is underway on the development of texture by solid state thermal gradient processing to produce textured superconducting oxides at high growth rates and development of models for, and experiments on, combustive oxidation including work on model systems.

314. RADIATION DISORDER AND APERIODICITY IN IRRADIATED CERAMICS
L. W. Hobbs, Department of Materials Science and Engineering
(617) 253-6835 01-4 $113,390

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

315. MICROSTRUCTURAL DESIGN IN CELLULAR MATERIALS
L. J. Gibson, Department of Civil Engineering
(617) 253-7107 01-5 $94,402

Investigation of efficient microstructures for cellular solids through micromechanical modeling and production of cellular materials with the proposed microstructures. Characterization of the microstructure and mechanical properties of the materials. Comparison of the models with the experimental data. Comparison of the efficiencies with the proposed microstructures.

316. CONSTRUCTION OF A SMALL ANGLE NEUTRON SCATTERING SPECTROMETER FOR INVESTIGATION OF MICROEMULSIONS AND MICELLAR SOLUTIONS IN BULK, IN POROUS MATERIALS AND UNDER SHEAR
S. -H. Chen, Department of Nuclear Engineering
(617) 253-3810 03-2 $110,000

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 ·th 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

317. MAGNETIC MULTILAYER INTERFACE ANISOTROPY
M. J. Pechan, Department of Physics
(513) 529-4518 02-2 $43,342

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

318. HIGH TEMPERATURE STABILITY, INTERFACE BONDING, AND MECHANICAL BEHAVIOR IN 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 $70,000

Investigation of the microstructural stability and mechanical properties of reinforced ordered intermetallic (primarily β-NiAl) (Al_2O_3 and SiC, particles, whiskers, and short fibers) interfacial bonding has been modified by an alumina coating applied by ion beam enhanced deposition. High temperature strength and low-temperature toughness will be measured.

319. THEORETICAL STUDIES OF BREAKDOWN IN RANDOM MEDIA
P. M. Duxbury, Department of Phyics and Astronomy
(517) 353-9179 01-3 $64,000

Scaling theories and numerical algorithms for predicting structure/extreme property relationships in random media. Use of concepts in statistical mechanics, disordered systems and nonequilibrium growth in conjunction with fracture mechanics, damage mechanics and dielectric breakdown to develop unified perspective of breakdown phenomena. Development of generic models and general methodology, and treatment of specific breakdown problems.

MICHIGAN TECHNOLOGICAL UNIVERSITY
Houghton, MI 49931

320. EFFECTS OF GRADIENTS ON BOUNDARY STABILITY
S. Hackney, Department of Metallurgical Engineering
(906) 487-2170 01-1 $148,600

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

UNIVERSITY OF MICHIGAN
Ann Arbor, MI 48109-2136

321. FUNDAMENTAL ALLOY DESIGN OF OXIDE CERAMICS AND THEIR COMPOSITES
I. -W. Chen, Department of Materials Science and Engineering
(313) 763-6661 01-2 $95,642

Three alloy design approaches to oxide ceramics for structural and energy applications. Aliovalent ions in solid solutions investigated for space charge segregation and effects on grain growth, dislocation creep and intergranular cavitation. Precipitation of spinel-based layers compounds studied for toughened and strengthened composites. Ceramic matrix composites with interpenetrating ductile phase prepared by infiltration of porous ceramic preforms with liquid under pressure. Structure property relationships established through variation of microchemical, microstructural, crystallographic, and other material parameters.

322. THE ROLE OF GRAIN BOUNDARY CHARACTER IN THE ENVIRONMENTALLY-ASSISTED INTERGRANULAR CRACKING MECHANISM OF NICKEL-BASE ALLOYS
G. S. Was, Department of Nuclear Engineering
(313) 763-4675 01-2 $134,799

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).

323. THE STRUCTURAL BASIS FOR FATIGUE INITIATION IN GLASSY POLYMERS
A. F. Yee, Department of Materials Science and Engineering
(313) 764-4312 01-2 $136,799

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.

324. A FREE ENERGY SIMULATION METHOD BASED STUDY OF INTERFACIAL SEGREGATION
D. J. Srolovitz, Department of Materials Science and Engineering
(313) 936-1740 01-3 $128,180

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.

325. SYNCHROTRON STUDIES OF NARROW BAND MATERIALS
J. W. Allen, Department of Physics
(313) 763-1150 02-2 $100,000

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 high temperature superconductivity materials, including metal-insulator transitions. Data to be analyzed using density-functional calculations and many-body Hamiltonian models.

326. NONEQUILIBRIUM AND NONLINEAR EFFECTS IN GROWTH
L. M. Sander, Department of Physics
(313) 764-4471

R. Savit, Department of Physics
(313) 764-4437 02-3 $191,867

A new approach to understand 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

327. 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 $71,018

Research to address: (1) crack dynamics and inherent plasticity effects, (2) ligament contributions to fracture resistance and (3) micro-mechanics of final instability. Polycrystalline and single crystal materials investigated as a function of temperature, grain size and material thickness. Materials: Fe-3wt%Si single crystals, Au and Ir. Techniques include detailed fractography, acoustic emission, selected area channeling pattern (SACP) evaluation, cleavage modeling, TEM, impact and mechanical studies, AES, XPS, SIMS, UPS, EELS, and STM.

328. THEORETICAL STUDY OF REACTIONS AT THE ELECTRODE-ELECTROLYTE INTERFACE
J. W. Halley, Department of Physics and Astronomy
(612) 624-0395 01-3 $119,718 (18 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.

329. FUNDAMENTAL STUDIES OF STRESS DISTRIBUTIONS AND STRESS RELAXATION IN OXIDE SCALES ON HIGH TEMPERATURE ALLOYS
D. A. Shores, Department of Chemical Engineering and Materials Science
(612) 625-0014 01-3 $178,430

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

330. MODELING AND EXPERIMENTAL STUDIES OF OXIDE COVERED METAL SURFACES
W. H. Smyrl, Department of Chemical Engineering and Materials Science
(612) 625-0717 01-3 $341,055

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.

331. THEORY OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF SOLID STATE OXIDES
J. R. Chelikowsky, Department of Chemical Engineering and Materials Science
(612) 625-4837 02-2 $69,000

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 65201

332. HIGH PRESSURE OPTICAL STUDIES OF SEMICONDUCTORS AND HETEROSTRUCTURES
H. R. Chandrasekhar, Department of Physics and Astronomy
(314) 882-6086 02-2 $59,852

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

333. INELASTIC SCATTERING WITH HIGH INTENSITY MOSSBAUER RADIATION
W. B. Yelon, Department of Physics
(314) 882-5236 02-2 $88,694 (9 months)

This project aims at the development and use of ultra high intensity Mossbauer sources for scattering experiments. The technique has been shown to be feasible and it has been applied to the investigation of the precise character of the resonance line shape, anharmonicity in sodium, diffusive properties of organic liquids, and critical phenomena in charge density wave layer compounds. Studies have been initiated in soft modes, phasons and interference with potential applications in testing possible violation of time reversal invariance in the electromagnetic decay of nuclei. The work is being carried out at the University of Missouri Research Reactor Facility and with a specially constructured scattering facility at Purdue University. Both conventional and conversion electron scattering techniques are being used, particularly microfoil conversion electron (MICE) detectors to enhance signal-to-off-resonance counting rates.

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

334. THEORETICAL STUDIES ON THE ELECTRONIC STRUCTURE AND PROPERTIES OF CERAMIC CRYSTALS AND GLASSES
W. -Y. Ching, Department of Physics
(816) 235-2503 01-1 $105,572

Calculation by means of orthogonalized linear combination of atomic obitals (OLCAO) of electronic structure and linear optical properties for a larger number of oxide, nitride, phosphate, silicate, III-V semiconductors, metallic glass and high-T_c superconducting materials. 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.

UNIVERSITY OF MISSOURI AT ROLLA
Rolla, MO 65401

335. ELECTRONIC TRANSPORT AND MIXED CONDUCTIVITY IN PEROVSKITE
H. U. Anderson, Department of Ceramic Engineering
(314) 341-4886 01-3 $113,300

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

336. ELECTROACTIVE POLYMERS AND LIQUID CRYSTALS
V. H. Schmidt, Department of Physics
(406) 994-6173 03-2 $53,100

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.

NATIONAL ACADEMY OF SCIENCES
2101 Constitution Avenue
Washington, D.C. 20418

337. PANEL ON ASSESSMENT OF SELF-ASSEMBLING AND BIOMOLECULAR MATERIALS
R. Taylor
(202) 334-3520 03-2 $15,000

Partial support of the Solid State Sciences Committee of the National Academy of Sciences to provide studies and addressment of funding needs and educational concerns of the field of materials science and engineering in the academic, industrial, and government sectors.

UNIVERSITY OF NEBRASKA
Lincoln, NE 68588-0111

338. FUNDAMENTAL STUDIES OF STRONGLY MAGNETIC RARE-EARTH-TRANSITION METAL ALLOYS
D. J. Sellmyer, Department of Physics
(402) 472-2407 02-2 $60,000

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

UNIVERSITY OF NEVADA
Reno, NV 89557

339. PHOTOPHYSICAL PROPERTIES OF TRIPLET EXCITATIONS ON POLYMERIC SYSTEMS
R. D. Burkhart, Department of Chemistry
(702) 784-6041 03-1 $91,895

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 nonplanar to assess the extent to which structural modifications can influence rates of exciton migration. Modification of the rate of triplet-triplet annihilation by microwave-induced mixing, monitor the dependence of triplet quantum yields on the energy of excitation, and to probe the direct detection of carbazole radical cations by transient absorption spectroscopy.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 87131

340. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE SILICATES, COMPLEX OXIDES, AND PHOSPHATES
R. C. Ewing, Department of Geology
(505) 277-4163 01-1 $123,729

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 (XANES). Materials studied include zircon ($ZrSiSiO_4$), thorite/huttonite ($ThSiO_4$), monazite ($CePO_4$), titanite ($CaTiSiO_5$), and uraninite (UO_2).

341. ADSORPTION STUDIES AT A SOLID-LIQUID INTERFACE
J. A. Panitz, Deparment of Physics
(505) 277-8488 01-1 $154,055

Adsorption phenomena at a solid-liquid interface. Monolayer films and multilayer structures formed on metal and semiconductor surfaces by Langmuir-Blodgett and simple diffusive adsorption from aqueous solution. Surface morphology, adsorbate conformation, and chemical analysis of interface mapped in high vacuum on a subnanometer scale using a new instrument that combines high-resolution transmission electron microscopy with imaging atom-probe mass spectroscopy. Vitreous ice, formed from the native environment, used to cryoprotect the interface, allowing the embedded interface and the species adsorbed on its surface to be transferred into high vacuum for analysis without modification or damage.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27695

342. STRUCTURE-PROCESSING-PROPERTY RELATIONS IN COPPER OXIDE-BASED HIGH-T_c SUPERCONDUCTORS
A. I. Kingon, Department of Materials Science and Engineering
(919) 515-7907 01-1 $123,634

Investigate relationships between the crystallographic and electronic structure of copper oxide-based compounds and their electronic and superconducting properties. Fundamental understanding of the parameters determining the structure of the copper-oxygen sublattice. Study of aspects controlling grain boundary composition to provide structure-properties relationship.

343. CRACK GROWTH RESISTANCE BEHAVIOR IN v TOUGHENED CERAMICS
R. O. Scattergood, Department of Materials Science and Engineering
(919) 515-7843 01-5 $115,723

Systematic study of fundamental aspects of erosion and impact damage in brittle materials and advanced ceramic systems. Materials investigated include aluminas, fiber-reinforced ceramics, transformation-toughened ceramics and various model brittle materials. New or modified apparatus designed and constructed for particle properties and threshold effects. Experimental results on erosion behavior and impact damage utilized for new fracture-mechanics analyses and erosion models development. Erosion rates vs. particle sizes, velocities and impact angles. Characterization of microstructural, strength and fracture properties. Erodent particle properties influence on nature of threshold effects.

344. RESEARCH AT AND OPERATION OF THE MATERIAL SCIENCE X-RAY ABSORPTION BEAMLINE (X-11) AT THE NATIONAL SYNCHROTRON LIGHT SOURCE
D. E. Sayers, Department of Physics
(919) 515-3482 02-2 $339,713

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

345. BAND ELECTRONIC STRUCTURES AND CRYSTAL PACKING FORCES
M. H. Whangbo, Department of Chemistry
(919) 515-3464 03-1 $98,696

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

346. THEORETICAL STUDIES OF SURFACE REACTION ON METALS AND ELECTRONIC MATERIALS
J. L. Whitten, Department of Chemistry
(919) 515-7277 03-1 $70,000

Theoretical studies of the adsorption of small molecules and molecular fragments on the surfaces of nickel and silicon using the embedding formulation of ad initio calculations. Energy contours and preferred surface adsorption sites are calculated along with vibrational frequencies for adsorbates. In some cases, excited electronic states will be calculated to help sort out the direct ionization vs. Auger processes that relate to electron or photon stimulated desorption from silicon surfaces. The embedding scheme is uniquely suited to these computations.

UNIVERSITY OF NORTH CAROLINA
Chapel Hill, NC 27514

347. SOLID-STATE VOLTAMMETRY AND SENSORS IN GASES AND OTHER NON-IONIC MEDIA
R. W. Murray, Department of Chemistry
(919) 962-6295 03-2 $52,000 (10 months)

Miniaturized electrochemical cells suitable for electrochemical voltammetry of electroactive materials dissolved in or affixed to thin ionically conducting polymer films have been designed and tested. The cells are based on microdisk electrodes sealed in glass capillaries or are fashioned as microband electrodes microlithographically. Experiments with these cells are aimed at developing a range of electrochemical methodologies, with appropriate boundary value theory, to bring the diagnostic power developed for electrochemical voltammetry in fluid electrolytes to rigid polymeric media experiments. Secondly, the polymer solvent film can be exposed to a bathing gas whose consitituents can interact in a plasticizing or in a chemically reactive way with the polymer solution, altering the observed electrochemical voltammetry. Such interactions presently form the basis for investigation of the molecular aspects of polymer plasticization effects and chemical reactivity in polymer phases, and may be applied to design sensors for bathing gas constituents.

NORTHWESTERN UNIVERSITY
Evanston, IL 60208

348. DEFECT CLUSTERING IN SIMPLE AND COMPLEX OXIDES
T. O. Mason, Department of Materials Science and Engineering
(708) 491-3198

D. E. Ellis, Department of Physics and Astronomy
(708) 491-3665 01-1 $207,690

Study of defect clustering and related properties of oxides involving transport and nonstoichiometry measurements, diffraction, microscopy, and quantum theoretical methods. Oxides of interest include highly defective transition metal monoxides (Fe, MnO, CoO, NiO), transition metal spinels (Fe_3O_4 and Mn_3O_4), stabilized ZrO_2, and ternary systems, such as $Ca_xNi_{1-x}O$ and high-T_c superconductors. Transport and nonstoichiometry studies in a high oxygen potential cell that permits substantially higher defect concentrations to be achieved. Structural and valence studies by X-ray and neutron diffraction, electron microscopy, and near-edge absorption spectroscopy. Finite temperature modeling (using molecular dynamic and statistical mechanics approaches) of defects in monoxides and total energy calculations of defect arrangements in complex oxides. Modeling of defect dependent properties of materials.

349. ATOMIC STRUCTURE AND COMPOSITION OF INTERNAL INTERFACES
D. N. Seidman, Department of Materials Science and Engineering
(708) 491-4391 01-1 $113,447

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

350. TRANSFORMATION PLASTICITY IN DUCTILE SOLIDS
G. B. Olson, Department of Materials Science and Engineering
(708) 491-2847 01-2 $157,760

Mechanisms of transformation toughening in ductile solids investigated by: (a) detailed observations of crack-tip processes, and (b) numerical modeling with experimentally-derived constitutive relations. Model alloy steels (γ'-strengthened and phosphocarbide strengthened steels) used to study room temperature transformation toughening and constitutive behavior. Shear-instability-controlled fracture observed at sectional crack-tips with and without transformation plasticity interactions using alloy composition to vary phase stability. Quantitative constitutive relation for experimental alloys applied to crack-tip and notch fields to study transformation plasticity interaction with various models of microvoid-softening-induced shear localization.

351. STUDY OF MECHANICAL BEHAVIOR AND INTERNAL STRUCTURE OF FERRITIC NANOCRYSTALLINE MATERIAL
J. R. Weertman, Department of Materials Science and Engineering
(708) 491-7823 01-2 $92,731

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.

352. PLASMA, PHOTON, AND BEAM SYNTHESIS OF DIAMOND FILMS
R. P. H. Chang, Department of Materials Science and Engineering
(708) 491-3598 01-3 $98,147

Deposition of polycrystalline diamond films with hydrogen plasma; effects of process conditions, including gas pressure, charged species in plasma, metallic and ceramic substrates, surface chemistry, role of interfacial layer in promoting adhesion; film structure, graphite inclusion. Investigation of gas phase nucleation of diamond particles.

353. DEFECT STRUCTURE OF SEMICONDUCTING AND INSULATING EPITAXIAL OXIDES
B. W. Wessels, Department of Materials Sciences and Engineering
(312) 491-3219 01-3 $98,669

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, photoluminescence, Hall effect measurements and transmission electron microscopy; optical and electronic properties and thermal stability of defects determined.

354. THE EFFECT OF MOISTURE ON THE MICROSTRUCTURE OF CEMENT-BASED MATERIALS
H. Jennings, Department of Civil Engineering
(708) 491-4858 01-5 $133,000 (16 months)

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.

355. ENERGETICS, BONDING AND ELECTRONIC STRUCTURE OF METAL/CERAMIC INTERFACES
A. J. Freeman, Department of Physics and Astronomy
(708) 491-8639 02-3 $109,576

Model the energetics, bonding, bonding mechanism and structure of metal/ceramic interfaces. Investigate surface electronic structure of oxides and interface grain-boundaries in transition metal-simple oxide interfaces, e.g., Pd and Nb alumina interfaces as well as metal/SiC interfaces. Investigations of ferroelectricity in lead titanate and antiferroelectricity in lead zirconate. Investigations of the electronic structure of TiO_2 surfaces and the properties and structures of VO_2/TiO_2 interface.

356. MIXED IONIC AND ELECTRONIC CONDUCTIVITY IN POLYMERS
M. A. Ratner, Department of Physics
(708) 491-5655

D. F. Shriver, Department of Physics
(708) 491-5655 03-2 $101,500

This proposal is an investigation of ionic transport along and through interfaces, both within a given solid electrode or electrolyte and between solid electrodes and electrolytes. The objective is mechanistic understanding of which processes result in overpotential, degradation, charge accumulation, and enhanced mobility at such interfaces. Two general classes of materials will be investigated: siloxane based polymer electrolytes, and layered chalcogenide cathods. Experiments will include synthesis and surface modification of electrolyte films, bulk and interfacial impedance measurements, and simulation of interfacial transport phenomena by Monte Carlo and percolation theory techniques.

357. STRUCTURE SHEAR RESPONSE AND TRANSFER PROPERTIES OF LIPID MONOLAYERS
P. Dutta, Department of Physics
(708) 491-5465

J. B. Ketterson, Department of Physics
(708) 491-5468 03-3 $104,000

Study the mechanical properties of organic monolayers on the surface of water (Langmuir films). Determine the microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) using ellipsometry, conventional and synchrotron X-rays. Mechanical property studies directed toward shear response, and important but previously neglected structural property. Diffraction technique, involving external reflection at the monolayer surface, used to determine film structure. Use standing-wave fluorscence technique to determine the distribution of ions in the aqueous phase near the head groups in lipid monolayer films.

UNIVERSITY OF NOTRE DAME
Notre Dame, IN 46556

358. SINGLE-ELECTRON TUNNELING
S. T. Ruggiero, Department of Physics
(219) 239-7463 02-2 $58,391

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

OHIO STATE UNIVERSITY
Columbus, OH 43210

359. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT IMPERFECT BOUNDARIES SEPARATING ANISOTROPIC MATERIALS
L. Adler, Department of Welding Engineering
(614) 292-1974 01-5 $98,600

Fundamental research program on nondestructive characterization of internal defects in anisotropic materials. Specific activities include modeling of two-dimensional crystal imperfections using the finite boundary stiffness approach and acoustic microscopy.

360. THE HYDROGEN INDUCED STRESS CORROSION CRACKING OF NICKEL BASE ALLOYS IN HIGH TEMPERATURE WAVES
S. Smialowska, Department of Materials Engineering
(614) 292-0290 01-5 $117,757

Research intended to explain the intergranular stress corrosion cracking mechanism for nickel and iron base alloys in deaerated water at high temperatures. Examination of the role played in IGSCC by metallic constituents in both fcc and bcc alloys. Determination of the entry of hydrogen at anodic potentials as a result of chemical reactions. Dissolution rates of metallic constituents of alloys and distribution of cations between oxide films and water solutions. Ellipsometric and AES studies to determine thickness, roughness, and chemical composition of oxide films as they change, depending upon the alloy and conditions of exposure. X-ray diffraction measurements at 300-350 C in situ to determine if structural changes occur in alloys in zones where a large amount of hydrogen accumulates. TEM used to differentiate bubbles formed by methane from voids caused by creep. Effects of hydrogen carbonates on film formation.

361. EXOTIC SUPERCONDUCTING AND NORMAL STATES OF HEAVY ELECTRON AND HIGH-T_c MATERIALS
D. Cox, Department of Physics
(614) 292-0620 02-3 $60,000 (8 months)

Quadropole fluctuation mediated superconductivity in heavy electron systems. Investigation of the effect of quadrupolar fluctuations on the superconductivity of UBe_{13}. Application of self consistent conserving approximations to Anderson Lattice Models of heavy electron systems. Exploration of quadrupolar fluctuation induced superconductivity in the four band Anderson Lattice Model.

362. STRONGLY INTERACTING FERMION SYSTEMS
J. W. Wilkins, Department of Physics
(614) 292-5193 02-3 $165,000

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.

363. NEW CARBOHYDRATE-BASED MATERIALS
M. R. Callstrom, Department of Chemistry
(614) 292-0917   03-1 $70,000 (14 months)

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.

364. MOLECULAR FERROMAGNETISM
A. J. Epstein, Department of Physics
(614) 292-1133

J. S. Miller, Central Res. & Development Dept.
E. I. duPont de Nemours & Co.
Wilmington, DE 19898
(302) 695-1199   03-1 $165,606

Study of cooperative magnetic behavior and its microscopic origins in molecular and polymeric materials. Synthesis and characterization of novel ferromagnets and elucidation of the origins of ferromagnetic exchange. Objective is to develop design criteria for the synthesis of new ferromagnetic materials possessing desirable physical properties including high temperature transitions to a ferromagnetic state. Study of magnetism in molecular ferromagnets and origins of the ferromagnetic exchange. Synthesis of $(M(C_5(CH_3)_5)_2)^+$ and $(M(C_6R_6)^+$ (M=Cr,Fe,Ru, and Ni) salts of planar radical anions 7,7,8,8-tetracyanoquinodimethane (TCNQ), tetracyanoethiene (TCNE), and 2,3-dichloro-5,6 dicyanobenzoquinone (DDQ). Measurements of magnetism as a function of field, temperature, and pressure and comparison of results with models of one-dimensional ferro-ferrimagnetism. Mossbauer spectroscopy measurements for internal magnetic fields, spectroscopic measurements for charge transfer bands and inelastic neutron scattering measurements for magnetic structure.

OHIO UNIVERSITY
Athens, OH 45701

365. ELECTRONIC STATES IN SYSTEMS OF REDUCED DIMENSIONALITY
S. E. Ulloa, Department of Physics and Astronomy
(614) 593-1729   02-3 $51,000

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

366. RHEO-OPTICAL STUDIES OF MODEL "HARD SPHERE" SUSPENSIONS
B. J. Ackerson, Department of Physics
(405) 744-5819   01-3 $61,342

Spontaneous and artifically induced microstructure of particles in suspensions of hard spheres; effect the microstructure on macroscopic properties. Interparticle ordered induced by shear flows and rheological properties; use of velocimetry techniques to determine microscopic flow properties; microstructure induced by sedimentation with and without shear; growth rate of hard sphere crystals.

OREGON STATE UNIVERSITY
Corvallis, OR 97331

367. HYPERFINE EXPERIMENTAL INVESTIGATION OF ZIRCONIA CERAMICS
J. A. Gardner, Department of Physics
(503) 737-3278   01-1 $110,497

Perturbed angular correlation (PAC) spectroscopy of nuclear gamma rays to investigate Zr-containing ceramics. PAC characterization of free energies, transformation mechanisms, equilibrium phase boundaries, diffusion and relaxation models, short range order, order-disorder reactions, and elevated-temperature/time dependent effects in various zirconia-based ceramics that contain either Hf-181 or In-111 as a probe. Investigation of Zr-91 in zirconia by nuclear quadrupole resonance (NQR) and of O-17 substituted zirconia by nuclear magnetic resonance (NMR). NQR/NMR experiments to complement and expand the studies of local structure and oxygen vacancy dynamics underway with PAC.

UNIVERSITY OF OREGON
Eugene, OR 97403-0237

368. SURFACE AND INTERFACE ELECTRONIC STRUCTURE
S. D. Kevan, Department of Physics
(503) 346-4742 02-2 $140,000

Experimental characterization of the electronic structure of clean and adsorbate-covered metal surfaces using high resolution angle resolved photoemission spectroscopy at the National Synchrotron Light Source. Emphasis is on relativistic effects on surface electronic and geometric structures, determination of Fermi surfaces for surface localized states, and characterization of resonant electronic states. Metals to be investigated include the 4d and 5d transition metals.

369. MONITORING INTERFACIAL DYNAMICS BY PULSED LASER TECHNIQUES
G. L. Richmond, Department of Chemistry
(503) 686-4635 03-2 $105,204

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
University Park, PA 16802

370. GRAIN-BOUNDARIES
J. S. Lannin, Department of Physics
(814) 865-9231 01-1 $93,670

Study of clusters and cluster-assembled ultrathin films and interfaces. Measurements of the influence of deposition conditions, substrate system, influence of hydrogen on substrate and film properties and changes in film deposition conditions. Characterization techniques include Raman scattering, ultraviolet photoemission spectroscopy, Auger spectroscopy, fiber optic-based ellipsometry and transmission electron microscopy. Research on elemental semimetallic, metallic and semiconducting systems; elements include Sb, C, Sn, and Bi.

371. THE MECHANICAL BEHAVIOR OF SURFACE MODIFIED CERAMICS
D. J. Green, College of Earth and Mineral Sciences
(814) 863-2011 01-2 $80,000

Modification of surface layers of ceramics to introduce surface compression and increase hardness and fracture toughness of transformation toughened ZrO_2 and Al_2O_3. Surface infiltration when ceramic is pressed or partially sintered. Development of a second phase surface layer during final densification. Indentation cracking used to study crack nucleation and growth and determine fracture toughness. Stress and composition profiles determined by NSLS X-ray diffraction data.

372. TWIN BOUNDARIES, INTERFACES AND MODULATED STRUCTURES IN MARTENSITES
G. R. Barsch, Materials Research Laboratory
(814) 865-1657 01-3 $20,000

Theoretical study with concurrent supporting experimental investigations on coherent and semicoherent interfaces in ferroelastic martensites, including twin boundaries and twin bands, interfaces, modulated structures, and transformation precursors. Motivation is the need for a new theoretical basis for investigating the martensite nucleation mechanism and for establishing the conditions for nonclassical nucleation. Study of soliton-like solutions of a dynamic Ginzburg-Landau continuum theory for ferroelastic martensites in order to determine the strain distribution and strain energy for various geometric configurations as a function of the materials parameters, temperature and external stress. Model parameters of the theory consist of the second and higher order elastic constants and the harmonic strain gradient coefficients in the parent phase. Elastic and inelastic neutron scattering and X-ray measurements of the transformation strain versus temperature. Simultaneous ultrasonic velocity and attenuation measurements on biaxially stressed crystals in $In_{1-x}Tl_x$ alloys in order to determine the second and higher order elastic constants in the single domain tetragonal state. Special attention is given to transformation precursors in the cubic parent phase in order to eliminate their effect on the model parameters.

373. FUNDAMENTAL STUDIES OF PASSIVITY AND PASSIVITY BREAKDOWN
D. D. MacDonald, Department of Earth and Mineral Sciences
(814) 863-7772 01-3 $180,332

Study of the effects of minor alloying elements on passivity breakdown and of photo effects on properties of passive films. Use of electrochemical and phtoelectrochemical 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 suceptibilities of existing alloys to pitting corrosion.

374. INFLUENCE OF POINT DEFECTS ON GRAIN-BOUNDARY DIFFUSION IN OXIDES
V. S. Stubican, Department of Materials Science and Engineering
(814) 865-9921 01-3 $70,000

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.

375. INTERFACIAL PHENOMENA IN LASER WELDING
T. DebRoy, Department of Materials Science and Engineering
(814) 865-1974 01-5 $190,654

Improved composition control and properties of weld metal through basic understanding of interfacial chemistry and control of interstitial impurities. Dissolution of nitrogen, oxygen, and hydrogen in weld metal under simulated and actual welding conditions. Improved physical understanding of the dynamics of liquid metal ejection during laser welding. Incorporation of improved interfacial physics and chemistry in numerical simulation of weld pool mass transfer. Parameters affecting mass transfer. Ongoing collaborative program with Oak Ridge National Laboratory.

376. AN INVESTIGATION OF THE STRUCTURE AND PHASE RELATIONS OF C-S-H GELS
M. W. Grutzeck, Materials Research Laboratory
(814) 863-2779 01-5 $132,000 (18 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.

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

S. Komarneni, Materials Research Laboratrory
(814) 865-1542 03-2 $78,000

Synthesis and characterization of crystalline materials formed at low temperatures by topotactic and epitactic routes. The objective is to apply some of the very new and exciting advances in chemically-bonded ceramics to making much stronger and more impermeable materials that can be processed at low temperatures. The material has potential application as low-level radioactive waste hosts.

UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

378. STRUCTURE AND DYNAMICS IN LOW-DIMENSIONAL GUEST-HOST SOLIDS
J. E. Fischer, Deparment of Materials Science and Engineering
(215) 898-6924 01-1 $167,948

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

379. ATOMISTIC STUDIES OF GRAIN-BOUNDARIES IN ALLOYS AND COMPOUNDS
V. Vitek, Department of Materials Science and Engineering
(215) 898-7883 01-1 $153,390

Atomistic computer simulation studies of grain-boundaries in binary ordered and disordered alloys. Investigation of grain-boundaries with segregated solutes. Examination of the relationship between grain-boundary structure and surfaces formed by fracturing along these boundaries. Study of grain-boundary electronic structure. Methods of calculation of interatomic forces. Ni_3Al, Cu_3Au, CuAu, and NiAl are candidate alloys to be studied.

380. 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 $157,429

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 deformations, and the incompatibility of deformation at the boundary. Monotonic and cyclic experiments will focus on copper bicrystals and slip line analysis and TEM will be combined with continuum methods. Behavior of copper compared to Cu-Al having different stacking fault energy and a planar slip mode.

381. CONDENSED MATTER PHYSICS AT SURFACES AND INTERFACES OF SOLIDS
E. J. Mele, Department of Physics
(215) 898-3135 02-3 $65,000

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

382. MICROSTRUCTURE AND MAGNETIC PROPERTIES IN HIGH-ENERGY PERMANENT MAGNETS
W. A. Soffa, Department of Materials and Engineering
(412) 624-9720 01-3 $112,646

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

383. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES
J. V. Maher, Department of Physics and Astronomy
(412) 624-9007 02-2 $120,000

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 where the length scale of the etchings are very well controlled and much smaller than the smallest length scale in the pattern. Three other experiments will study the underlying physics which determines the lower-length-scale selection in three distinctly difference 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.

384. COMPUTER SIMULATIONS FOR THE ADSORPTION OF POLYMERS AND SURFACES
A. C. Balazs, Department of Materials Science and Engineering
(412) 648-9250 03-2 $42,000

Computer simulations and theoretical models to examine how the self-association reactions of amphiphilic polymers affect surface adsorption. Of particular interest is understanding how the architecture of the polymer chain and conditions such as the nature of the surface or solvent affect the extent of adsorption and the morphology of the interfacial layers. By understanding the factors that affect adsorption, predictions of chain geometries and conditions will yield the optimal interfacial sturcture for such applications as steric stabilization, adhesion and film growth. The significant advantage of computer simulations is that currently they are the only "experimental" tool with which one can simultaneously visualize the geometry of these self-assembled chains in solution, the comformation of the chains adsorbed directly to the surface and the microstructure of the entire interfacial region.

POLYTECHNIC UNIVERSITY
Brooklyn, NY 11201

385. SCANNING TUNNELING MICROSPECTROSCOPY OF SOLIDS AND SURFACES
E. Wolf, Department of Physics
(718) 260-3080 02-2 $120,000

Development of Scanning Tunneling Microscopy (STM) techniques as applied to the study of solids and surfaces. Probe both normal and superconducting states of materials. Basic information about the new class of many-body states in heavy fermion materials. Pairing symmetry study of $La_{1.8}Sr_{0.2}CuO_4$ a new high temperature superconductor. Basic superconducting tunneling phenomena; Josephson and proximity effects. Importance of spin-orbit coupling arising from the f-electron character of the heavy quasiparticles in heavy fermion materials. Quasiparticle spectroscopy of exotic conductors including organic superconductors.

386. SHORT RANGE ORDER EFFECTS: CERIUM AND ACTINIDE MATERIALS
P. Riseborough, Department of Physics
(718) 260-3675 02-3 $66,700

Theoretical studies of the effects of strong electronic correlations on highly degenerate narrow band materials such as uranium and cesium based f band metals. Short range ordering that may occur as a result of local moment correlations using a 1/N expansion, where N is the degeneracy of the material. Similar techniques applied to high-T_c superconductors. Field dependence of the de Haas-van Alphen effect. Compton scattering and Angle Resolved Photoemission Spectra for the latter materials. Comparison of theory with these and other experimental observations.

PRINCETON UNIVERSITY
Princeton, NJ 08544

387. VISCOELASTICITY OF POLYMER MELTS
W. W. Graessley, Department of Chemical Engineering
(609) 258-5721 01-2 $135,000 (18 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.

388. THERMOCHEMISTRY OF PHASES RELATED TO OXIDE SUPERCONDUCTORS
A. Navrotsky, Department of Geological and Geophysical Sciences
(609) 258-4674 01-3 $108,460

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.

PURDUE UNIVERSITY
West Lafayette, IN 47907

389. BEAM LINE OPERATION AND MATERIALS RESEARCH UTILIZING NSLS
G. L. Liedl, Materials Engineering Division
(317) 494-4095 01-1 $310,923

A grant to support MATRIX, a group of scientists from several institutions who have common interests in upgrading and in utilizing X-ray synchrotron radiation for unique materials research. The group has available a specialized beam line at the National Synchrotron Light Source (NSLS). A unique and versatile monochromator provides radiation to a four-circle Huber diffractometer for the basic system. Multiple counting systems are available as well as a low temperature stage, a high temperature stage, and a specialized surface diffraction chamber. The grant covers the operational expenses and system upgrade of this beam line at NSLS for all MATRIX members, and to support part of the research on phase transformation studies, X-ray surface and interface studies.

390. STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA
H. Sato, School of Materials Engineering
(317) 494-4099 01-3 $93,670

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.

391. MIDWEST SUPERCONDUCTIVITY CONSORTIUM
A. I. Schindler, Department of Materials Engineering and Physics
(317) 494-5567 01-5 $2,945,318

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.

392. SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION
J. R. Mullen, Department of Physics
(317) 494-3031 02-2 $88,694 (9 months)

This project aims at the development and use of ultra high intensity Mossbauer sources for scattering experiments. The technique has been shown to be feasible and it has been applied to the investigation of the precise character of the resonance line shape, anharmonicity in sodium, diffusive properties of organic liquids, and critical phenomena in charge density wave layer compounds. Studies have been initiated in soft modes, phasons and interference with potential applications in testing possible violation of time reversal invariance in the electromagnetic decay of nuclei. The work is being carried out at the University of Missouri Research Reactor Facility and with a specially constructured scattering facility at Purdue University. Both conventional and conversion electron scattering techniques are being used, particularly microfoil conversion electron (MICE) detectors to enhance signal-to-off-resonance counting rates.

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

Investigation of the photo-excitation process at low photon energies. Techniques under development directly measure the excited state energy distribution of electrons that are emitted through the surface potential barrier. The fundamental process; photo-excitation of electrons from field emission tips by a focussed argon-ion laser beam tuned to operate at a specific photon energy. Measurement of localized surface states on semiconducting and polymeric materials. Laser-induced diffusion and desorption effects associated with illumination of adsorbate-covered, submicron surfaces. Exploration of advantages and properties of a laser-illuminated scanning tunneling microscope.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, NY 12180

394. MECHANISM OF MECHANICAL FATIGUE IN FUSED SILICA
M. Tomozawa, Department of Materials Engineering
(518) 276-6451 01-2 $93,670

Mechanism of cyclic fatigue and analysis of fatigue kinetics in fused silica. Measurement of diffusion coefficient and solubility of water in silica glass as a function of stress, temperature, and water vapor pressure. Preparation of silica glass containing various water contents. Effect of water content on swelling and mechanical property alteration. Effect of environment on crack initiation and propagation. Comparison of cyclic and static fatigue in various environments.

UNIVERSITY OF RHODE ISLAND
Kingston, RI 02881

395. SURFACE PHYSICS WITH COLD AND THERMAL NEUTRON REFLECTOMETRY
A. Steyerl, Department of Physics
(401) 792-2204 02-1 $75,691

It is proposed to extend the methods of surface reflectometry to the use of ultracold 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

396. ULTRATHIN MAGNETIC FILMS AND PARTICLE-SURFACE INTERACTIONS WITH SPIN-SENSITIVE ELECTRON SPECTROSCOPIES

G. K. Walters, Department of Physics
(713) 527-6046

F. B. Dunning, Department of Physics
(713) 527-3544   02-2 $220,000

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

UNIVERSITY OF ROCHESTER
Rochester, NY 14627

397. MICROSTRUCTURAL BEHAVIOR OF NONEQUILIBRIUM SYSTEMS

J. C. M. Li, Department of Mechanical Engineering
(716) 275-4038   01-2 $102,329

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 peening 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.

398. DYNAMICS OF SURFACE MELTING

H. E. Elsayed-Ali, Laboratory for Laser Energetics
(716) 275-5101   03-3 $96,000

Experimental study of the melting transition of metal single crystals focussing on the occurrence and nature of surface melting. Picosecond time resolved reflection high energy electron diffraction (RHEED) will be used as a surface structure probe. The fast time resolution will be used to examine the dynamical processes taking place during the melting transition. Picosecond laser heating will be employed. Initially, low index facets of lead, bismuth, zinc, and cadmium will be examined.

ROCKWELL INTERNATIONAL
Thousand Oaks, CA 91360

399. MECHANISMS OF MECHANICAL FATIGUE IN CERAMICS

B. N. Cox, Science Center
(805) 373-4128

D. B. Marshall, Science Center
(805) 373-4170   01-2 $123,161

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

RUTGERS STATE UNIVERSITY OF NEW JERSEY
Piscataway, NJ 08855

400. THERMODYNAMICS, KINETICS AND STRUCTURAL BEHAVIOR OF SYSTEMS WITH INTERMEDIATE PHASES
A. G. Khachaturyan, Department of Mechanics and Materials Science
(201) 932-4711

T. Tsakalakos, Rutgers, Department of Mechanics and Materials Science
(201) 932-4711 01-1 $108,000

Elastic strain energy of an arbitrary two-phase microstructure. Strain-induced interaction of finite elements of a precipitate phase. Microscopic nonlinear kinetic equations of diffusional ordering with *elastic strain contribution. Computer simulation* of the strain-induced mesoscale structure in Y-Ba-Cu high temperature superconducting oxides.

UNIVERSITY OF SOUTHERN CALIFORNIA
Los Angeles, CA 90089

401. TRANSFORMATION INDUCED DUCTILITY IN INTERMETALLIC ALLOYS
E. Goo, Department of Materials Science
(213) 743-0961 01-2 $40,000

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

402. SYNTHESIS OF NOVEL ASSOCIATING WATER-SOLUBLE COPOLYMERS
T. E. Hogen-Esch, Department of Chemistry
(213) 743-3798

E. J. Amis, Department of Chemistry
(213) 743-6913 03-1 $95,200

Synthesis of water-soluble acrylic and cellulosic copolymers based on perfluorocarbon- and polydimethyl-siloxane derivatives of acrylic comonomers in which the hydrophobe length and that of a flexible polyethylene oxide connecting *spacer to the acrylic group are systematically varied.* Structural features, important for enhancing the viscosity of aqueous solutions at very low polymer concentrations (<1000 ppm), will be investigated with dynamic light scattering, rheology, and solution dynamics. The potential for mobility control of water-soluble copolymers that cluster as a result of polyanion-polycation interactions will be explored.

SOUTHWEST RESEARCH INSTITUTE
San Antonio, TX 78284

403. CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION
R. A. Page, Department of Materials and Mechanics
(512) 522-3252

K. S. Chan, Department of Materials and Mechanics
(512) 522-2053 01-2 $124,235

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

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

M. Urquidi, Chemistry and Chemical Engineering Laboratories
(415) 859-3195 01-3 $176,955

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 94305-6060

405. MECHANICAL PROPERTIES OF MATERIALS WITH NANOMETER SCALE MICROSTRUCTURES
W. D. Nix, Department of Materials Science and Engineering
(415) 725-2605 01-2 $159,097

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

406. FUNDAMENTAL STUDIES OF THE CHEMICAL VAPOR COMPOSITION OF DIAMOND
D. A. Stevenson, Department of Materials Science and Engineering
(415) 723-4251 01-3 $123,250

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.

407. A STUDY OF MECHANICAL PROCESSING DAMAGE IN BRITTLE MATERIALS
B. T. Khuri-Yakub, Department of Electrical Engineering
(415) 723-0718 01-5 $60,000

Study of mechanical damage and surface residual stresses associated with mechanical processing of brittle materials. Study of how defects in the green state of ceramic components evolve. Also, machine damage on curved surfaces. Development of a theory for calculating the behavior of surface wave propagation on curved surfaces. Materials include silicon nitride, porous silicon, and a variety of ceramic materials.

408. ULTRA-LOW TEMPERATURE PROPERTIES OF AMORPHOUS SOLIDS
D. D. Osheroff, Department of Physics
(415) 723-4228 02-2 $140,000

The thermal and dielectric properties of disordered solids between 1 mK and 100 mK will be investigated. The nature and role of lattice defects-two level systems-in the behavior of amorphous solids will be examined. Current thermometer technology will be extended in the temperature range of interest through a systematic investigation of the ultra-low temperature behavior of the dielectric constant of glasses.

409. A QUEST FOR A NEW SUPERCONDUCTING STATE
J. P. Collman, Department of Chemistry
(415) 723-4648

W. A. Little, Department of Physics
(415) 723-4233 03-1 $212,000

Research is directed towards understanding the mechanism by which 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; these are being prepared by magnetron sputtering and laser ablation. Electrochemical experiments using superconducting films as electrodes are being studied around the superconducting critical temperature T_c. X-ray diffraction of copper-free, superconducting bismuthate materials are to be studied above and below T_c in search of a structural phase transition which may be related to the superconducting mechanism. A new technique, "distributed point contact proximity effect tunneling," is being developed to understand the mechanism underlining the high-T_c superconducting cuprates. New mesodiscotic porphyrin derivatives are being prepared; their solid state properties and structures will be studied.

STATE UNIVERSITY OF NEW YORK AT BUFFALO
Buffalo, NY 14214

410. SUNY BEAMLINE FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE
P. Coppens, Department of Chemistry
(716) 831-3911 02-2 $360,000

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.

411. X-RAY STUDIES OF MICROSTRUCTURES IN SEMICONDUCTORS AND SUPERCONDUCTING MATERIALS
Y. H. Kao, Department of Physics
(716) 636-2576 02-2 $110,000

Investigation of the short range order structure in semiconductors and high temperature superconducting materials. Experimental methods: X-ray fluorescence, absorption, scattering, and electron yield to probe the local environment surrounding impurity atoms, interfaces and depth profile of constituent atoms at the National Synchrotron Light Source at Brookhaven National Laboratory. High quality samples prepared and characterized by collaborators at IBM and Phillips Laboratories.

STATE UNIVERSITY OF NEW YORK AT STONY BROOK
Stony Brook, NY 11794

412. 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 $147,500

Chemisorbed metal adsorbates on metal surfaces. Investigate structure with low energy electron diffraction (LEED). Determine electron band structure, including valence band shifts with layer thickness, with ultraviolet photoemission spectroscopy (UPS) on the U-7 beam line at the National Synchrotron Light Source at the Brookhaven National Laboratory. Research divided into efforts on rare-earth metals, diatomic molecules on metal surfaces, surface and bulk alloys, noble metals, and thin films.

413. PHASE TRANSITION IN POLYMER BLENDS AND STRUCTURE OF IONOMERS
B. Chu, Department of Chemistry
(516) 632-7928 03-2 $100,000

Kinetics of phase separation in polymer solutions and blends. Structure of phase separated droplets. Size, shape, and distribution of micro domains measured using light and X-ray scattering, excimer fluorescence, and optical microscopy. Phase separation kinetics measured using time-resolved, small angle X-ray scattering at the National Synchrotron Light Source. Studies of polymer-solvent systems, such as polystyrene- methylacetate, and polymer-polymer blends, such as polystyrene blended with polyvinyl methyl ether, polyisoprene, or polyorthochlorostyrene. Structure of sulfonated polystyrene ionomers using SAXS.

UNIVERSITY OF TENNESSEE
Knoxville, TN 37996-0140

414. 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 $145,800 (14 months)

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

UNIVERSITY OF UTAH
Salt Lake City, UT 84112

415. 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 $96,410

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.

416. FABRICATION, PHASE TRANSFORMATION STUDIES, AND CHARACTERIZATION OF SIC-ALN-AL_2OC
A. V. Virkar, Department of Materials Science and Engineering
(801) 581-5396 01-1 $80,683

Analysis of phase equilibria and phase transformations and the relationship between creep behavior and microstructure in the SiC-AlN-Al_2OC system. Diffusional phase transformations leading to phase separation. Modulated microstructures developed by spinodal decomposition. Cellular precipitation. Dependence of creep behavior on composition and microstructure.

417. ALUMINA REINFORCED TETRAGONAL ZIRCONIA (TZP) COMPOSITES
D. K. Shetty, Department of Materials Science and Engineering
(801) 581-6449 01-2 $90,712

Transformation toughening and reinforcement in composites; modeling of dependence of fiber-matrix interfacial properties on thermal expansion mismatch and processing temperature with glass-matrix compositles; relationship between matrix cracking stress and interfacial properties. Effect of secondary additives on transformation toughening of Ce-TZP-alumina composites. Effects of fiber coatings on interfacial bonding and mechanical properties of alumina fiber-reinforced Y-TZP composites. Electrical-mechanical analog to evaluate stress-intensity factors for matrix cracks in fiber reinforced composites.

418. 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 $79,000

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, recombination processes, and resonant Raman spectroscopy. Time-resolved: femtosecond to nanosecond, CW photomodulation spectroscopy, and ultrasonic phonon spectroscopy.

VIRGINIA COMMONWEALTH UNIVERSITY
Richmond, VA 23284-2000

419. STRUCTURE, STABILITY AND SPECTROSCOPY OF METAL CLUSTERS
P. Jena, Department of Physics
(804) 367-1313

B. K. Rao, Department of Physics
(804) 257-1313 01-3 $165,560

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

420. CHARACTERIZATION OF SUPERCONDUCTING MATERIALS WITH MUON SPIN ROTATION
C. E. Stronach, Department of Physics
(804) 524-5915 01-3 $86,000 (7 months)

Use of muon spin rotation to characterize the magnetic states in high temperature and heavy-Fermion superconductors. Investigate the relationship between magnetic ordering and superconductivity.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

421. STUDY OF THE EMBEDDED ATOM METHOD OF ATOMISTIC CALCULATIONS FOR METALS AND ALLOYS
R. A. Johnson, Department of Materials Science
(804) 924-6356 01-1 $49,186

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

422. INITIAL STAGES OF GRAIN-BOUNDARY PRECIPITATION
G. J. Shiflet, Department of Materials Science
(804) 924-6340 01-1 $112,404

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

423. SURFACE STRUCTURE AND ANALYSIS WITH SCANNING TUNNELING MICROSCOPY AND ELECTRON TUNNELING SPECTROSCOPY
R. V. Coleman, Department of Physics
(804) 924-3781 02-2 $80,000 (6 months)

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

424. SUPERCONDUCTING MATERIALS
J. Ruvalds, Department of Physics
(804) 924-6796 02-3 $87,000

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 anomolous damping observed experimentally and calculated by the principal investigator. Normal state properties of the high temperature oxides will be investigated, including, e.g., reflectively, the Hall effect, electronic Raman scattering, and anomolous susceptibility.

WASHINGTON STATE UNIVERSITY
Pullman, WA 99164-5045

425. METAL INDUCED EMBRITTLEMENT
R. G. Hoagland, Department of Mechanical and Metallurgical Engineering
(509) 335-8280 01-2 $61,859

Study of metal-induced embrittlement. Crack growth measurements combined with microscopic examinations of fracture specimens to establish the relationship between crack extension and crystallographic orientation, to characterize competing crack-tip reactions, and to assess plastic wake effects. Computer simulations of embrittlement mechanisms on an atomic scale. Aluminum embrittled by mercury and gallium.

426. A STUDY OF TRANSIENT PARTICLE COARSENING
H. Hoyt, Department of Mechanical and Materials Engineering
(509) 335-8523 01-3 $72,000 (18 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.

WASHINGTON UNIVERSITY
St. Louis, MO 63130

427. MULTI-BODY FORCES AND ENERGETICS OF TRANSITION METALS, ALLOYS, AND SEMICONDUCTORS
A. E. Carlsson, Department of Physics
(314) 889-5739 02-3 $80,683

Development of computation methods for calculation of interatomic potentials used in simplified tight-binding models of transition metals and their alloys. Extension beyond the tight-binding model. Interatomic potentials tested both by experimental data and density-of-states band calculations. Applied to surfaces and vacancies and subsequently used to calculate phase diagrams and the properties of dislocations and grain-boundaries.

UNIVERSITY OF WASHINGTON
Seattle, WA 98195

428. X-RAY AND GAMMA-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE
R. L. Ingalls, Department of Physics
(206) 543-2778 02-2 $125,000

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.

429. THEORETICAL STANDARDS OF XAFS
J. J. Rehr, Department of Physics
(206) 543-8593 02-2 $51,323

A state-of-the-art computer code for theoretical simulations of X-ray absorption fine structure (XAFS) for use by the XAFS community will be developed. The code will be consistent with recommendations of the International Workshop on Standards and Criteria in X-ray absorption. The latest theoretical developments will be incorporated and the code will be compared with experiment to choose between alternative theoretical prescriptions. The code will incorporate multiple scattering effects. These are important in the study of complex materials.

430. LOCAL ENVIRONMENT INDUCED BY IMPURITIES
E. A. Stern, Department of Physics
(206) 543-2023 02-2 $19,220 (3 months)

Conduct a program of X-ray absorption (XAFS) and Mossbauer studies on the local changes induced when impurities are substituted in a Pb host. Confirm the circumstances under which a liquid-like bubble exists around the impurity, ascertain the extent to which the Lindemann criterion is applicable and detemine the relation between surface and bulk melting.

WEST VIRGINIA UNIVERSITY
Morgantown, WV 26506

431. ELECTRONIC AND MAGNETIC INTERACTIONS IN HIGH TEMPERATURE SUPERCONDUCTING AND HIGH COERCIVITY MATERIALS
B. R. Cooper, Department of Physics
(304) 293-3423 02-3 $66,000

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

UNIVERSITY OF WISCONSIN AT MADISON
Madison, WI 53706

432. THERMODYNAMICS, KINETICS, AND INTERFACE MORPHOLOGIES OF PHASE FORMATION REACTIONS BETWEEN METALS AND GALLIUM ARSENIDE: BULK VS THIN-FILM STUDIES
Y. A. Chang, Department of Materials Science and Engineering
(608) 262-1821 01-3 $88,540

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.

433. GRAIN-BOUNDARY STUDIES IN IONIC CONDUCTORS
E. E. Hellstrom, Department of Materials Sciences and Engineering
(608) 263-9462 01-3 $128,000 (18 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. Modeling of grain-boundary segregation and space-charge layer.

434. LOCALIZED-ITINERANT MAGNETISM: THIN FILMS AND HETEROSTRUCTURES
M. Onellion, Department of Physics
(608) 263-6829 02-2 $56,850 (9 months)

Application of the Magneto-Optic Kerr Effect (MOKE) with energies between 1.4 and 35 eV and electron spin polarization to the characterization of rare-earth films, rare-earth-transition metal bilayers and to chromium dioxide/cobalt heterostructures. Determine rare-earth core level anisotropy as a function of temperature and layer thickness. Investigate the orientation of magnetism in rare-earth thin films. Examine magnetic exchange interaction within and between layers in metal heterostructures.

435. MORPHOLOGICAL ANALYSIS OF IONOMERS
S. L. Cooper, Department of Chemical Engineering
(608) 262-4502 03-2 $108,480

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

436. INELASTIC ELECTRON SCATTERING FROM SURFACES
S. Y. Tong, Department of Physics
(414) 229-5765 02-3 $120,000

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

WORCESTER FOUNDATION FOR EXPERIMENTAL BIOLOGY
222 Maple Avenue
Shrewburgy, MA 01545

437. NOVEL BIOMATERIALS: GENETICALLY ENGINEERED PORES
H. P. Bayley
(508) 842-9146 03-2 $78,525

Recombinant DNA technology is being used to make a selection of microscopic porse by genetic manipulation of a bacterial channel protein. Pores with different internal diameters, with differential selectivity for the passage of classes of molecules (e.g., anions vs. cations), and different gating properties (the ability to open and close in response to a stimulus, e.g., electric field) will be made. Eventually these molecules might be incorporated into materials such as thin films to confer novel permeability properties upon them. The molecule being remodeled is hemolysin (HL), which is secreted by the common bacterium, Staphylococcus aureus. It comprises a single polypeptide chain of 33,200 daltons, of known sequence, capable of forming hexameric pores in membrances ~11.4A in internal diameter. Our specific aims are: 1) To obtain pure, active HL by expression of the HL gene in E. coli. 2) To locate the domain of HL responsible for pore formation using deletion mutagenesis. 3) To alter this domain by point mutagenesis to produce new pores with a range of properties. 4) To define the properties of these molecules using a combination of biochemical and biphysical techniques. HL has several advantage over other polypeptides that might be used in such a project. It is a small robust polypeptide that will be relatively easy to reengineer, and it can be obtained in gram amounts. The hexameric pore can be assembled from the monomer in vitro by the addition of an inexpensive detergent.

SECTION C

Small Business Innovation Research

ADELPHI TECHNOLOGY
285 Hamilton Avenue
Palo Alto, CA 94301

438. A SURFACE PLASMON MONITOR FOR IN-SITU THIN FILM ANALYSIS
E. Fontana
(415) 328-7337 Phase I SBIR $49,995

Surface plasmon resonance phenomenon used to eliminate limitations of conventional optical methods for thin-film thickness and surface structure monitoring. Demonstration of the capability to measure thin film optical constants, submicroscopic surface roughness, and thickness down to subangstrom dimensions. Multiparameter processing by use of relatively simple optical principles and low cost instrumentation. Feasibility of silver and gold films on glass substrates.

ADVANCED RESEARCH AND APPLICATIONS CORPORATION
425 Lakeside Drive
Sunnyvale, CA 94086

439. RAPID LIGHT ELEMENTAL ANALYSIS WITH TRANSMISSION ELECTRON MICROSCOPY
J. A. Kerner
(408) 733-7780 Phase I SBIR $50,000

Re-entrant light element X-ray fluorescence analyzer for analytical transmission electron microscopy (TEM) to be constructed and demonstrated to have improved efficiency over conventional wavelength dispersive instruments. Use of advanced X-ray optical components to collect and transport characteristic radiation; large solid-angle optics using X-ray multilayer coatings. Integration of TEM sample stage, boron collection optics and detector to form re-entrant analyzer; demonstration of improved efficiency for analysis of boron.

ADVANCED TECHNOLOGY MATERIALS, INC.
7 Commerce Drive
Danbury, CT 06776

440. SYNCHROTRON MONOCHROMATOR CRYSTAL GROWTH
D. Cummings
(203) 794-1100 Phase I SBIR $50,000

Growth of yttrium boride (YB_{66}) single crystals for soft X-ray spectroscopy; novel gradient temperature control. Several crystals of YB_{66} will be grown and characterized.

CERACON, INC.
1101 North Market Blvd.
Sacramento, CA 95834

441. NOVEL SUPERPLASTIC ALUMINUM ALLOYS BY CONTROLLED CRYSTALLIZATION OF GLASSY ALUMINUM ALLOYS
R. V. Raman
(916) 928-1933 Phase I SBIR $49,864

Controlled consolidation crystallization of glassy aluminum alloys to produce alloys with dual-structure, equiaxed, ultrafine grain matrix which is suitable for superplastic forming. Demonstration of feasibility of high-speed (seconds), high pressure (200,000 psi) rolling process to produce suitable alloys.

CONDUCTUS, INC.
969 Maude Avenue
Sunnyvale, CA 94086

442. X-RAY DETECTORS USING SUPERCONDUCTING TRANSITION METAL TUNNEL JUNCTIONS
J. M. Rowell
(408) 737-6705 Phase I SBIR $47,598

Development of superconductor-insulator-superconductor tunnel junction X-ray detectors; niobium-aluminum junction; multilayer electrodes for quasiparticle trapping. Low temperature measurement of leakage currents in junctions, determination of performance of most promising of junctions produced, design of optimum X-ray detector.

INRAD, INC.
181 Legrand Avenue
Northnale, NJ 07674

443. SINGLE CRYSTAL MOLYBDEUM MIRRORS FOR HIGH POWDER VACUUM ULTRAVIOLET AND X-RAY RADIATION
W. Ruderman
(201) 767-1910 Phase II SBIR $499,026

A process for producing high quality single crystals of molybdeum of large dimension will be investigated and a method for making very low scatter superpolished surfaces for such crystals will be sought. Representative molybdenum mirrors will be evaluated for crystal perfection; surface flatness, roughness and total integrated scatter; reflectivity as a function of wavelength from 5 eV to 30 eV; and laser damage threshold at 193 nm.

MULTILAYER OPTICS AND X-RAY TECHNOLOGY, INC.
7070 University Station
Provo, UT 84602

444. DEVELOPMENT OF FLEXIBLE SUPERLATTIC ARTIFICIAL CRYSTALS FOR USE IN FIXED-SOURCE JOHANN X-RAY SPECTROMETERS WITH APPLICATION TO ANALAYTICAL TRANSMISSION ELECTRON MICROSCOPY
M. Lund
(801) 378-3972 Phase II SBIR $500,000

An alternate implementation of the Johann spectrometer will be pursued which has a variable radius bent crystal. Techniques for making superlattice artificial wavelength dispersive crystals on flexible substrates will be developed and the resulting crystals tested.

NANOPHASE TECHNOLOGIES CORPORATION
8205 South Cass Ave.
Darien, IL 60559

445. NET SHAPE FORMING OF NANOPHASE CERAMICS FOR MECHANICAL APPLICATIONS
J. C. Parker
(708) 963-0282 Phase I SBIR $50,000

Demonstrate net shape forming of various nanophase ceramics; characterization of resulting shapes with respect to hardness, fracture toughness, porosity and mechanical strength; development of database on mechanical and modeling properties of nanophase ceramics. Metal oxide powders prepared by gas phase condensation process; consolidated into simple shapes at different temperatures and pressing conditions; property characterization.

NORTH STAR RESEARCH CORPORATION
5555 Zuni SE, Suite 345
Albuquerque, NM 87108

446. MATERIALS SYNTHESIS WITH HIGH-POWER COAXIAL PLASMA GUNS
R. J. Adler
(505) 296-3596 Phase I SBIR $49,800

Synthesis of nonequilibrium materials using high power, pulsed coaxial plasma guns, developed for DOE magnetic fusion and defense programs. Technical feasibility for novel alloy mixing of metastable materials for metallurgical and tribological applications. Evaluation of comprehensive databases for potential materials processing applications; conduct of materials processing to measure symmetry, power flow, and energy coupling; development of system studies to judge the technical, economical and envrionmental feasibility of the method.

PEAK INSTRUMENTS, INC.
112 W. Franklin Avenue
Pennington, NJ 08534

447. AN EFFICIENT X-RAY WAVELENGTH SPECTROMETER FOR IMPROVED ELEMENTAL ANLAYSIS ON THE ANALYTICAL ELECTRON MICROSCOPE
N. C. Barbi
(609) 737-8133 Phase II SBIR $399,601

A new type of wavelength dispersive (WD) X-ray spectrometer is proposed. Its anticipated attributes of high efficiency and small physical size make it suitable for use on Analytical Electron Microscope (AEMs), where current WD spectrometers are generally inappropriate. Preliminary calculations indicate that the efficiency of the new device should be, at low angles, about equal to a 200 mm Rowland circle Bragg spectrometer for the same crystal; at high angles, the new device may be up to 1000 times more efficient. Compared to energy dispersive (ED) specrometers commonly used on AEMs, the proposed WD spectrometer should provide more sensitive analysis, particularly for the light elements (with atomic numbers less than 10).

SYNERGETIC MATERIALS, INC.
P. O. Box 5574
Auburn, CA 95604

448. PLASTIC BEHAVIOR AND PROPERTIES OF TITANIUM CARBIDE AND TITANIUM CARBONITRIDE MONOLITHIC AND COMPOSITE MATERIALS

D. C. Halverson
(916) 823-0238 Phase I SBIR $50,000

Plastic behavior and property-microstructure relationships in titanium carbide (TIC) and titanium carbonitride (TICN) materials. Monlithic TIC and TICN ceramics synthesized using self-propagating high temperature synthesis (SHS); TIC-metal and TICN-metal composites synthesized using SHS and liquid metal infiltration (LMI). Microhardness, macrohardness, fracture toughness; microstructure evaluation using metallographic, X-ray diffraction and electron microprobe analysis.

SECTION D

Major User Facilities

(Large Capital Investment)

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, New York 11973

The National Synchrotron Light Source (NSLS) is the nation's largest facility dedicated to the production of synchrotron radiation. The facility has two electron storage rings: a vacuum ultraviolet ring which operates at an electron energy of 750 meV and an X-ray ring which operates at 2.5 GeV. The bending magnet sources on these rings provide useable photon fluxes from 0.01 to 1.0 keV and 1.0 to 20.0 keV, respectively. These bending magnets are the source for the 30 X-ray ports and 17 VUV ports. By further sharing of these sources, as many as four beamlines can be accommodated on a single port, providing the NSLS facility with a capacity to run approximately 100 experiments simultaneously. By the end of 1990, the Light Source had 79 operational beamlines conducting experiments.

From their conception, the designs of the storage rings included long, field free straight sections for special radiation sources (wigglers and undulators). The two straight sections on the VUV ring and the five available on the X-ray ring now have a variety of wigglers and undulators providing radiation that is anywhere from one to several orders of magnitude brighter than the comparable bending magnets. These devices are the sources for a wide variety of experiments in the biological, chemical, and materials sciences. The first General User programs using insertion device beamlines began in FY 1991.

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. By August 30, 1991, 2590 scientists from 376 universities, laboratories, corporations, and foreign institutions were registered at the Light Source. This is an increase of 761 Users and 84 institutions from October 1990.

Proprietary research can be performed at the NSLS. The DOE has granted the NSLS a Class Waiver under whose terms the Proprietary User is obligated to pay the full cost recovery rate for NSLS usage. In return, the user has the option to take title to any inventions made during the proprietary research program and to treat as proprietary all technical data generated during the proprietary research program. In FY 1991, the total number of corporations participating in proprietary research at the Light Source was ten.

USER MODES

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in establishment of comprehensive long-range experimental programs. In addition to the beamlines constructed by the NSLS staff for general usage, a large number of beamlines have been designed and instrumented by Participating Research Teams (PRTs). The PRTs are entitled to up to 75 percent of their beamline(s) operational time for a 3-year term.

Insertion Device Teams (IDTs) have been formed to design, fabricate, commission, and use wiggler and undulator beamlines. The conditions and terms are similar to those of the PRTs.

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

A program is available to support faculty/student research groups performing experiments at the NSLS. The program is designed to encourage new users of these facilities and defray expenses incurred during exploratory visits to BNL, and while conducting initial experiments at the NSLS. It is aimed at university users having only limited grant support for their research. Approximately 85 faculty/student research members will have participated in this program by the end of FY 1991.

PERSON TO CONTACT FOR INFORMATION

Susan White-DePace
User Administration Office
NSLS, Bldg. 725D
Brookhaven National Laboratory
Upton, NY 11973

(516) 282-7114
FTS 666-7114

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bnl::swd
swd@bnl.gov

NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

TECHNICAL DATA

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

RESEARCH AREA	WAVELENGTH RANGE (Å)	NUMBER OF INSTRUMENTS
Circular Dichroism	1400 - 6000	1
Energy Dispersive Diffraction	0.1 - 2.5	3
EXAFS, NEXAFS, SEXAFS	0.1 - 250	24
Gas Phase Spectroscopy/ Atomic Physics	0.6 - 14.6	3
Infrared Spectroscopy	$2.5 \times 10^4 - 1.2 \times 10^6$	2
Lithography/Microscopy/Tomography	0.6 - 15	6
Medical Research	0.37	1
Nuclear Physics	$2.5 \times 10^{-6} - 2.5 \times 10^{-4}$	1
Photoionization	0.6 - 12000	5
Radiometry		1
Reflectometry	20 - 55	1
Research & Development/ Diagnostics	white beam	11
Time Resolved Fluorescence	1000 - 12000	2
Topography	0.1 - 3	3
Transverse Optical Klystron	12.5 - 1250	1
VUV & X-ray Photoemission Spectroscopy	0.3 - 1280	27
X-ray Crystallography	0.3 - 6.2	9
X-ray Fluorescence	0.3 - 20	2
X-ray Scattering/Diffraction	0.1 - 15.5	26

HIGH FLUX BEAM REACTOR

Brookhaven National Laboratory
Upton, New York 11973

The Brookhaven High Flux Beam Reactor (HFBR) presently operates at a power of 30 megawatts and provides an intense source of thermal neutrons (total thermal flux = 1.0×10^{15} neutrons/cm^2-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($\gamma > 4$ A). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure is also available. The emphasis of the research efforts at the HFBR has been on the study of fundamental problems in the fields of solid state and nuclear physics and in structural chemistry and biology.

USER MODE

Experiments are selected on the basis of scientific merit by a Program Advisory Committee (PAC), composed of the specialists in relevant disciplines from both within and outside BNL. Use of the facilities is divided between Participating Research Teams (PRT's) and general users. PRT's consist of scientists from BNL or other government laboratories, universities, and industrial labs who have a common interest in developing and using beam facilities at the HFBR. In return for their development and management of these facilities, each PRT is assigned up to 75 percent of the available beam time, with the remainder being reserved for general users. The PAC reviews the use of the facilities by the PRT's and general users and assigns priorities as required.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/ student research groups performing experiments at the National Synchrotron Light Source or at the HFBR. It is aimed at university users having limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

Rae Greenberg (516) 282-5564
Bldg. 510A FTS 666-5564
Brookhaven National Laboratory
Upton, NY 11973

HIGH FLUX BEAM REACTOR (continued)

TECHNICAL DATA

INSTRUMENTS	PURPOSE AND DESCRIPTION
5 Triple-axis Spectrometers (H4M, H4S, H7, H8, H9A)	Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 MeV, < E_o < 200 MeV Q range: 0.03 < Q < 10_{A-1}
Small Angle Neutron Scattering (H9B)	Studies of large molecules. Located on cold source with 20 x 20 cm^2 position-sensitive area detector. Sample detector distance L < 2 meter. Incident wavelength 4 Å < λ_o < 10 Å
Diffractometer (H3A)	Protein crystallography 20 x 20 cm^2 area detector λ_o = 1.57 Å
Small Angle Scattering (H3B)	Studies of small angle diffraction of membranes. Double multilayer monochromator 1.5 Å < λ < 4.0 Å 2d detector with time slicing electronics and on-line data analysis.
2 Diffractometers (H6S, H6M)	Single-crystal elastic scattering 4-circle goniometer 1.69 Å < λ_o < 0.65 Å
1 Triple-axis Spectrometer (H5)	Inelastic scattering Diffuse scattering Powder diffractometry
2 Spectrometers (H1A, H1B)	Neutron capture studies Energy range: 0.025 eV < E_o < 25 KeV
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.
Instruments - Soon to be Commissioned	
Neutron Reflectometer	Accommodates liquid or solid samples up to 40 cm long. .0025$Å^{-1}$≤Q≤0.25$Å^{-1}$, with resolution 1 x $10^{-3}Å^{-1}$. Reflection range 1-10^{-6}.
High Resolution Neutron Powder Diffractometer. (H1A1)	Determination of moderately complex crystalline structures. λ = 1.88Å, Δd/d = 5 x 10^{-4}Ge(511) vertical focussing monochromator. 64 He^3 detectors, covering 160 degrees.

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 4×10^{15} neutrons/cm^2-sec, and the flux at the inner end of the beam tubes is slightly less than 10^{15} n/cm^2-sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Facilities are available for studies of materials at low and high temperatures, high pressures, and high magnetic fields.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an external review committee. It is expected that all accepted experiments will be scheduled within 6 months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be borne by the user. Inexperienced users will normally collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full cost recovery, including a charge for beam time. A brochure describing the facilities and a booklet giving user procedures is available on request.

PERSON TO CONTACT FOR INFORMATION

R. M. Nicklow Solid State Division Oak Ridge National Laboratory Oak Ridge, Tennessee 37831-6393	(615) 574-5240 FTS 624-5240	Wide Angle
G. D. Wignall Solid State Division Oak Ridge National Laboratory 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 - 10^7n/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 = 1.015 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 Powder Diffractometer, Beam size - 5 x 3.7 cm, Wavelength = 1.4 angstroms, 32 detectors with 6 min collimators
HB-4SANS	Small-Angle Scattering Facility, Beam size - 3 cm diameter max, Wavelength = 4.75 or 2.38 angstroms, 10^4 - 10^6 n/cm^{2}s depending on slit sizes and wavelength, area detector 64 x 64 cm^2, sample to dector distance 1.5 - 19 m

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 with the installation of the new target is 1×10^{15} n/cm^2 sec. The source has some unique characteristics that have opened up new scientific opportunities:

- o high fluxes of epithermal neutrons (0.1-10 eV)
- o pulsed nature, suitable for real-time studies and measurements under extreme environment
- 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, it is expected that the facilities will be used for technological applications, such as stress distribution in materials and characterization of zeolites, ceramics, polymers, and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS, Building 360, Argonne National Laboratory. Neutron time for proprietary research can be purchased based on the full-cost recovery rate.

PERSONS TO CONTACT FOR INFORMATION

B. S. Brown, Division Director Argonne National Laboratory 9700 South Cass Avenue Argonne, IL 60439	(708) 252-4999 FTS 252-4999 FAX (708) 252-4163
T. G. Worlton, Scientific Secretary	(708) 252-8755 FTS 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)	2-20	**	2%	**	
Low-Res. Medium-Energy Chopper Spectrometer (C.-K. Loong)	0.1-30	0-0.6	0.02 k_o	0.05 E_o	
High-Res. Medium-Energy Chopper Spectrometer (C.-K. Loong)	0.3-9	0-0.4	0.01 k_o	0.02 E_o	
Small Angle Diffractometer (J. E. Epperson/P. Thiyagarajan)	0.006-0.35	**	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)	0.0-0.25	**	0.001	**	
Quasi-Elastic Neutron Spectrometer Spectrometer (F. Trouw)	0.42-2.59	0-0.1	~0.2	0.02 E_o	
Glass, Liquid and Amorphous Materials Diffractometer † (D. L. Price)	0.05-25 01-45	** **	~0.5% cotθ ~1.0% cotθ	** **	**
High Intensity Powder Diffractometer (F. Trouw)	0.5-25	**	1.8-3.5%	**	

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

Not Yet in the User Program

Small Angle Neutron Diffractometer (SAND, formerly SAD II, under development)

LOS ALAMOS NEUTRON SCATTERING CENTER

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The Los Alamos Neutron Scattering Center (LANSCE) facility is a pulsed spallation neutron source equipped with time-of-flight (TOF) spectrometers for condensed-matter research. Neutrons are produced by spallation when a pulsed 800-MeV proton beam, provided by the Los Alamos Meson Physics Facility (LAMPF) and an associated Proton Storage Ring (PSR), impinges on a tungsten target. To date, the PSR has achieved 75 percent of its design goal of 100-μA average proton current at 20-Hz repetition rate. At this level, LANSCE has the world's highest, peak thermal flux for neutron scattering research.

Current research programs at LANSCE use the following instruments: a filter difference spectrometer (FDS) for vibrational spectroscopy by inelastic neutron scattering; a Laue-TOF single-crystal diffractometer (SCD); a high-intensity powder diffractometer (HIPD) for structural studies of liquids, amorphous materials, and crystalline powders; a neutron powder diffractometer (NPD) with the highest resolution in the U.S.; a constant-Q spectrometer (CQS) for the study of collective excitations, such as phonons and magnons; a low-Q diffractometer (LQD) for small-angle scattering studies; and a surface profile reflectrometer (SPEAR) for studies of surface structure.

During the next 3 to 4 years, several new spectrometers will be installed at LANSCE, including: a chopper spectrometer for inelastic scattering measurements and Brillouin scattering and a back-scattering spectrometer with a resolution of 10 μeV or better.

USER MODE

LANSCE provides neutron scattering facilities for several communities. At least 80 percent of available beam time is used for condensed-matter research, while the remaining 20 percent is intended for internal use in support of the Laboratory's programmatic mission. Of the time available for condensed- matter work, most is distributed to a formal user program, which started in April 1988. Advice on experiments to be performed in this category is provided by a Program Advisory Committee (PAC) held jointly with the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory. Scientists based at universities, national laboratories, and industry may apply for beam time by submitting short proposals for scrutiny by the PAC. No charge is made for non-proprietary research.

CONTACT FOR USER INFORMATION

Maria DiStravolo
LANSCE Scientific Coordination and Liaison Office
Mail Stop H805
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-6069 or
FTS 843-6069

LANSCE (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 ($n/cm^2.S$)	1.7×10^{16}

INSTRUMENTS

32-m Neutron Powder Diffractometer (J. Goldstone, Responsible)	Powder Diffraction Wave vector 0.3-50 $Å^{-1}$ Resolution 0.13%
Single Crystal Diffractometer (A. Larson, Responsible)	Laue time-of-flight diffractometer Wave vectors 1-15 $Å^{-1}$ Resolution 2% typical
Filter Difference Spectrometer (J. Eckert, Responsible)	Inelastic neutron scattering, vibrational spectroscopy Energy trans. 15-600 meV Resolution 5-7%
High Intensity Powder Diffractometer (R. VonDreele, Responsible)	Powder diffraction .7% resolution; liquids and amorphous materials diffraction 2% resolution
Constant-Q Spectrometer (R. Robinson, Responsible)	Elementary excitations in single crystal samples Energy resolution 1-3%
Low Q Diffractometer (P. A. Seeger, Responsible)	Small angle scattering at a liquid hydrogen cold source Wave vectors 0.003-1.0 $Å^{-1}$
Reflectometer (G. Smith, Responsible)	Surface reflection at grazing incidence. Wave vector range 0.007 to 0.3 $Å^{-1}$

STANFORD SYNCHROTRON RADIATION LABORATORY

Stanford University
Stanford, California 94309-0210

SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research in biology, chemistry, engineering, geology, materials science, medicine and physics. In addition to scientific research utilizing synchrotron radiation the Laboratory program includes the development of advanced sources of synchrotron radiation (e.g., insertion devices for the enhancement of synchrotron radiation as well as modifications of SPEAR). SSRL presently 23 has experimental stations. The radiation on 11 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. Non-invasive angiography. Soft X-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter. X-ray lithography and microscopy. SSRL serves approximately 650 scientists from 114 institutions working on over 150 active proposals. A wide variety of experimental equipment is available for the user and there are no charges either for use of the beam or for the facility-owned support equipment. Proprietary research may be performed on a cost-recovery basis by special arrangement.

USER MODE

SSRL is a user-oriented facility which welcomes proposals for experiments from all qualified scientists. SSRL operates for users 7-8 months per year. Over 75 percent of the beam time is available for the general user. Access is gained through proposal submittal and peer review. An annual Activity Report is available on request. It includes progress reports on about 100 experiments plus descriptions of recent facility developments. The booklets "Proposal Submittal and Scheduling Procedures" and "SSRL Experimental Stations" detail information on proposal submittal and experimental station characteristics.

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell (415) 926-3191
SSRL, Bin 69 PO Box 4349 FTS 462-3191
Stanford, CA 94309-0210

SECTION E

Other User Facilities

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The National Center for Small-Angle Scattering Research (NCSASR) is supported by the National Science Foundation and the Department of Energy under an interagency agreement. The two main instruments available to users are the NSF-constructed 30-m small-angle neutron scattering facility (SANS) and the DOE-constructed 10-m small-angle X-ray scattering camera (SAXS). These instruments are intended to provide state-of-the-art capability for investigating structures of condensed matter on a global scale, e.g., from a few tens to several hundreds of angstroms. They are intended to serve the needs of scientists in the areas of biology, polymer science, chemistry, metallurgy and materials science, and solid state physics.

USER MODE

Beam time on these instruments is assigned, in general, on the basis of proposals submitted in advance. These are then reviewed by a panel of experts external to the Laboratory and are rated on the basis of scientific merit. When a favorable review has been received, a staff member of the NCSASR and the user agree, usually by telephone, on a time and duration for the experiment. Ordinary charges are borne by the Center, but extensive use of support facilities (shops, computing, etc.) must be paid by the user. Users may work in collaboration with one or more staff members if they wish, but such collaboration is not required. Proprietary experiments can be carried out after contractual agreement has been reached.

PERSONS TO CONTACT FOR INFORMATION

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

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

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

TECHNICAL DATA

30-m SANS Instrument Specifications

Monochromator:	six pairs of pyrolytic graphite crystals
Incident wavelength:	4.75 angstroms or 2.38 angstroms
Wavelength resolution:	$\Delta\lambda/\lambda = 6\%$
Source-to-sample distance:	1.5-7.5 m
Beam size at specimen:	0.5-3.0 cm diam
Sample-to-detector distance:	1.5-19 m
K range:	$2 \times 10^{-3} < K_2 = 4\pi\lambda^{-1} \sin\theta < 0.6$ angstroms^{-1}
Detector:	64 by 64 cm^2
Flux at specimen:	10^4-10^6 n/cm^{2}s depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator:	hot-pressed pyrolytic graphite
Incident wavelengths:	1.542 angstroms (CuK α) or 0.707 angstroms (MoKα)
Source-to-sample distances:	0.5 - 5.0 m in 0.5 m intervals
Beam size at specimen:	0.2 cm diameter
Sample-to-detector distances:	1.0 - 5.0 m in 0.5 m intervals
K range covered:	$3 \times 10^{-3} \leq K \leq 0.6$ angstroms^{-1} (CuK α) $6 \times 10^{-3} \leq K \leq 1.2$ angstroms^{-1} (MoK α)
Flux at specimen:	10^6-10^7 photons per second depending on source-sample-detector distances
Detector:	20- by 20-cm^2 (electronic resolution 0.1 by 0.1 cm^2)
Special features:	Time slicing in periods as short as 10 seconds for transient relaxation experiments and interactive graphics for data analysis

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory Electron Microscopy Center for Materials Research provides unique facilities which combine the techniques of high- voltage electron microscopy, ion-beam modification, and ion-beam analysis, along with analytical electron microscopy.

The cornerstone of the Center is a High Voltage Electron Microscope (an improved Kratos/AEI EM7) with a maximum voltage of 1.2 MV. This HVEM is interfaced to two accelerators, a National Electrostics 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 100 CXII transmission and scanning transmission electron microscope (TEM/STEM) equipped with an X-ray energy dispersive spectrometer (XEDS), a Philips EM 420 TEM/STEM equipped with XEDS and an electron energy loss spectrometer (EELS) and a Philips CM30 with XEDS. Procurement of an advanced Analytical Electron Microscope (AEM) is underway. This state-of-the-art, field emission gun ultra-high vacuum AEM will operate up to 300 keV and have the highest available microanalytical resolution with capabilities for XEDS, EELS, and Auger Electron Spectroscopy AES. As such, it will have substantially increased analytical capabilities for materials research over present-day instruments.

USER MODE

The HVEM-Tandem Facility is operated as a national resource for materials research. Qualified scientists wishing to conduct experiments using the HVEM/TANDEM facilities of the Center should submit a proposal to the person(s) named below. Experiments are approved by a Steering Committee following peer evaluation of the proposals. There are no use charges for basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

PERSON(S) TO CONTACT FOR INFORMATION

C. W. Allen (708) 252-4157
and FTS 252-5222
E. A. Ryan (708) 252-5075
Electron Microscopy Center for Materials Res. FTS 252-5075
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 Kratos/AEI EM7 (1.2 MeV)	Resolution 9 Å pt-pt Continuous voltage selection (100-1200 kv) Current density 15 A/cm^2 High-vacuum specimen chamber Negative-ion trap Electron and ion dosimetry systems Video recording system Ion-beam interface Specimen stages 10 - 1300 K Straining and environmental stages
Transmission Electron Microscope JEOL 100 CX (100 keV)	Resolution 7 Å pt-pt Equipped with STEM, XEDS Specimen stages 85 - 900 K
Transmission Electron Microscope Philips EM 420 (120 keV)	Resolution 4.5 Å pt-pt Equipped with EELS, XEDS Specimen stages 30 - 1300 K
Transmission Electron Microscope Philips CM 30 (300 keV)	Resolution 2.5 Å pt-pt Equipped with XEDS Specimen stages 30 - 1300 K
High Resolution Electron Microscope JEOL 4000 EXII (400 kV)	Resolution 1.65 Å pt-pt Specimen stages RT
Analytical Electron Microscope Being procured (300 keV)	Resolution 2.8 Å pt-pt Ultra-high vacuum, Field Emission Gun Equipped with EELS, XEDS, AES, SIMS, LEED, etc. Specimen stages 85 - 1300 K

ACCELERATORS	
NEC Model 2 UDHS	Terminal voltage 2 MV Energy stability ± 250 eV Current density: H^+, 10 $\mu A/cm^2$ (typical) Ni^+, 3 $\mu A/cm^2$
NEC 650 kV Injector Being acquired	Terminal voltage 650 kV Energy stability ± 60 eV Current density: He^+, 100 $\mu A/cm^2$ (typical) Ar^+, 10 $\mu A/cm^2$

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

A wide range of facilities for use in materials science are available for collaborative research by members of universities or industry with ORNL staff members. The facilities include state-of-the-art electron microscopy, high voltage electron microscopy, atom probe/field ion microscopy, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include analytical electron microscopy (energy dispersive X-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS), and convergent beam electron diffraction (CBED)). Surface analysis facilities include four Auger electron spectroscopy (AES) systems, and 0.4, 2.0, and 5.0 Van de Graaff accelerators for Rutherford back-scattering and nuclear reaction techniques. Other equipment includes a mechanical properties microprobe (NanoIndenter), X-ray diffraction systems, rapid solidification apparatus, and various other facilities in the Metals and Ceramics Division.

USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, K. B. Alexender, G. M. Pharr, M. G. Burke, and N. D. Evans. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and current ORNL research. One ORNL staff member must be identified who is familiar with required techniques and will share responsibility for the project.

The SHaRE program provides technical help and limited travel expenses for academic participants through the Oak Ridge Associated Universities (ORAU).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik Metals and Ceramics Division Oak Ridge National Laboratory P. O. Box 2008 Oak Ridge, Tennessee 37831	(615) 574-5066 FTS 624-5066
A. Wohlpart Oak Ridge Associated Universities P. O. Box 117 Oak Ridge, Tennessee 37831	(615) 576-3422 FTS 626-3422

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

TECHNICAL DATA

Facilities	Key Capabilities	Applications
Philips EM400T/ FEG(AEM) 120 kV	EDS, EELS, CBED, STEM; minimum probe diam ~1 nm*	Structural and elemental microanalysis
Philips CM12 AEM 120kV	EDS, CBED, STEM;*	Structural and elemental microanalysis
JEOL 2000FX AEM 200 kV	EDS, CBED, EELS, STEM; examination of irradiated materials	Structural and elemental microanalysis
Philips CM30 AEM 300kV	EDS, (P) EELS, CBED, STEM;	Structural and elemental microanalysis
JEM 120C TEM 120 kV	Polepiece for TEM of ferromagnetic materials	Structural analysis
Atom Probe Field-Ion microscopes	TOF atom probe, imaging atom probe, FIM, pulsed laser atom probe	Atomic resolution imaging: single atom analysis elemental mapping
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam; fracture stage; RGA; depth profiling elemental mapping	Surface analytical and segregation studies
Varian Scanning Auger Electron Spectroscopy System	5 micron beam; hot-cold fracture stage; RGA: depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Triple Ion-Beam Accelerator Facilities	400 kV, 2 MV, 5 MV Van de Graff accelerators sputter profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis
Mechanical Properties Microprobe-Nanoindenter	Computer-controlled diamond indenter	High spatial resolution (0.1 μm lateral and 0.2 nm depth) measurements of elastic/plastic behavior

* Video recording; stages for cooling, heating, and deformation available for Philips microscopes.

CENTER FOR MICROANALYSIS OF MATERIALS

Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

The Center operates a wide range of advanced microchemistry, surface chemistry, electron microscopy, X-ray and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, micro- crystallography, surface analysis, structure, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded from the MRL, DOE, and NSF contracts, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff. The Center welcomes *external users from National Laboratories, Universities, and Industry.*

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research with a faculty member associated with the MRL. Independent usage by trained individuals is also encouraged. Assistance and collaboration with the professional staff of the Center is arranged as required. In all cases, the research carried out by users of the Center has to be in the furtherance of DOE objectives.

The equipment is made available on a flexible schedule. Professional help by the Center staff will be arranged to assist the users. Fully qualified users can and do use the equipment at any time of day.

The Center staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

In addition to the main items listed opposite, the Center also has also equipment: optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including ion-milling stations, a micro-ion mill, electropolishing units, sputter coaters, a spark cutter, ultrasonic cutter, diamond saw, dimpler, etc.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217)-333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

CENTER FOR MICROANALYSIS OF MATERIALS (continued)

INSTRUMENTS	'ACRONYM'	FEATURES AND CHARACTERISTICS
Imaging Secondary Ion Microprobe Cameca IMS 5f	SIMS	Dual ion sources (C_s^+, O_2^+). 1 µm resolution.
Secondary Neutral Mass Spectrometer Leybold Heraeus INA 3	SNMS	Quantitative analysis, Depth profiling.
Scanning Auger Microprobe Physical Electronics 595	Auger	Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector.
Scanning Auger Microprobe Physical Electronics 660	Auger	Resolution: SEM 25 nm Auger 60 nm
X-ray Photoelectron Spectrometer Electronics 5400	XPS	Resolution: 50 meV, 180° Physical spherical analyzer, Mg/Al and Mg/Ag anodes
X-ray Photoelectron Spectrometer Surface Science	XPS	Spherical analyzer, small spot size, gas doping, high temperature
Transmission Electron Microscope Philips EM430 (300kV)	TEM	Heating and cooling stages
Transmission Electron Microscope Philips EM420 (120kV) Stage (30K).	TEM	EDS (windowless), EELS, STEM, Cathodoluminescence, Cold
Transmission Electron Microscope Philips EM400T (120kV)	TEM	EDS. Heating, cooling stages
Transmission Electron Microscope Philips CM12 (120 kV)	TEM	High Resolution Analytic facilities
Transmission Electron Microscope JEOL 4000EX (400 kV)	TEM	For environmental cell use. Straining stages, heating stages
Transmission Electron Microscope Hitachi 9000 (modified)	TEM	0.16 nm resolution atomic imaging
Scanning Transmission E.M. Vacuum Generators HB5 (100kV)	STEM	0.5 nm probe, field emission gun, EDS, EELS.
Scanning Electronic Microscope Hitachi S800	SEM	Field Emission Gun Resolution 2nm, EDX
Scanning Electron Microscope EDX, JEOL JSM 35C (35kV)	SEM	5 nm resolution, channeling and backscattering patterns. High temperature deformation.
Scanning Electron Microscope Zeiss 960	SEM	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 Elliott 14 kW high brilliance source Rigaku 12 kW source Several conventional sources Rigaku D/Max-11B Computer Controlled Powder Diffractometer	X-ray	4-circle diffractometer. Small angle camera. EXAFS. Lang topography, Powder cameras, etc. High temperature and low temperature stages.
Proton Induced X-ray Emission	PIXE	*Quantitative chemical analysis*
Van de Graff Accelerator for electrons and ions		3 MeV accelerator Rutherford Backscattering Electron radiation damage Ion radiation damage

SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

This program utilizes a new approach for fundamental materials research. Ion implantation doping, ion-induced mixing, and other ion beam based techniques are utilized to alter the near-surface properties of a wide range of solids under vacuum conditions. In situ analyses by ion beam, surface, and bulk properties techniques are used to determine the fundamental materials interactions leading to these property changes. Since ion implantation doping is a nonequilibrium processes, it can be used to produce new and often unique materials properties not possible with equilibrium processing. Ion beam techniques are also useful to modify surface properties for practical applications in areas such as friction, wear, corrosion, catalysis, surface hardness, solar cells, semiconducting devices, superconductors, etc.

This program has emphasis on long-range basic research. Consequently, most cooperative research involving scientists from industries, universities, and other laboratories has been the investigation of new materials properties possible with these processing techniques or the determination of the mechanisms responsible for observed property changes. In many instances such research projects identify definite practical applications and accelerate the transfer of these materials alteration techniques to processing applications.

COOPERATIVE RESEARCH

User interactions are through mutually agreeable research projects between users and research scientists at ORNL which utilize the unique alteration/analysis capabilities of the SMAC facility. It should be emphasized that the goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application and not to provide routine service alterations or analyses.

PERSON TO CONTACT FOR INFORMATION

S. P. Withrow — (615) 576-6719
Solid State Division — FTS 626-6719
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6048

SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER

TECHNICAL DATA

ACCELERATORS	OPERATING CHARACTERISTICS
2.5-MV positive ion Van de Graaf	0.1-3.2 MeV; H, O, ^4He, ^3He, and selected gases. Beam current 100 nA
1.7-MV tandem	0.2-3.5 MeV H; 0.2-5.1 MeV ^3He, ^4He; negative ion sputtering source for heavy ion beams of selected 7 MeV
10-200-KV high-current ion implantation accelerator	Most ion species; 100-1000 microamps singly charged, microamps doubly and triply charged ~100
80-500-kV high-current ion implantation accelerator	Most ion species from microamp to milliamp current

FACILITIES	
UHV analysis chambers	Several chambers; vacuums 10^{-6}-10^{-11} torr; multiple access ports; UHV goniometers (4-1300K)
In situ analysis capabilities	Ion scattering, ion channeling, and ion-induced nuclear reactions; LEED, Auger, ion-induced Auger; electrical resistivity vs. temperature
Scanning electron microscope	JEOL-840 with energy dispersive X-ray analysis
Rapid thermal annealer	AG Heatpulse Model 410, with programmable, multistep heating to 1200° C.

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94551-0969

Optical techniques, primarily Raman spectroscopy and nonlinear optical spectroscopy, are being developed and used to study the behavior of materials exposed to high-temperature environments. 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.

Nonlinear optical spectroscopies, in particular second harmonic generation, have been developed for the detection of monolayer and submonolayer coverages of surfaces. Picosecond Nd:YAG and dye lasers (10 pps) and a high repetition rate (1kHz) Nd:YAG laser provide pulsed excitation at a variety of wavelengths. Extension of capabilities to the sub-hundred-femtosecond range is available. 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 diagostic approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the persons listed below. If further investigations appear reasonable, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government laboratories have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSONS TO CONTACT FOR INFORMATION

R. H. Stulen, Advanced Materials Research Division (8342)	(510) 294-2070 FTS 234-2070
Gary B. Drummond, Ass't to the Director (8301) Sandia National Laboratories Livermore, California 94551-0969	(510) 294-2697 FTS 234-2697

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

TECHNICAL DATA

INSTRUMENTS	KEY FEATURES	COMMENTS
Raman Surface Analysis System	UHV Chamber; Raman system with Ar laser; triple spectrograph, diode array detector and 2-D imaging photon counting detector; Auger; sputtering capability.	Simultaneous Raman and sputtering. Raman system capable of detecting 2 nm thick oxides. Sample heating up to 1100 C.
Raman Microprobe	Hot stage; Raman system with Ar, Kr lasers; scanning triple spectrometer.	1-2 micron spatial resolution. Hot stage can handle corrosive gases.
Raman High-Temperature Corrosion System	Furnace; Raman system with Ar, Kr, Cu-vapor lasers Nd:YAG; triple spectrograph and diode array detector.	Pulsed lasers gated detection for blackbody background rejection. Furnace allows exposure to oxidizing, reducing, and sulfidizing environments.
Combustion Flow Reactors	Raman system with Ar, Kr, Cu-vapor. lasers; triple spectrograph and diode array detector.	Vapor and particulate injection into flames. Real-time measurements of deposit formation.
Linear and Non-Linear Optical Spectroscopy of Electrochemical Systems	Electrochemical cell; Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and diode array detector; Nd:YAG laser, 1 Hz rep. rate.	Electrochemical cell with recirculating pump and nitrogen purge; Monolayer and submonolayer detection of metals, oxygen, and hydrogen adsorption at electrodes.
Nonlinear Optical Spectroscopy of Surfaces System	Picosecond Nd:YAG and dye lasers, 10 Hz; UHV chamber equipped with LEED, Auger, sputtering, and quad. mass spectroscopy; 100-ns pulse length, 10 Hz Nd:YAG laser.	Monolayer and submonolayer detection of high temperature hydrogen and oxygen adsorption and nitrogen segregation on alloys; laser thermal disorption.
Nonlinear Optical Spectroscopy of Electrochemical Systems	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.

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 Frederick A. Schmidt, Director, Materials Preparation Center.

Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquiries should be directed to Tom Wessels, MRSH Manager, (515) 294-8900.

High-T_c Superconductivity Information Exchange

The newsletter, High-T_c Update, is published twice-monthly and available without charge as either hard copy or electronic mail. Inquiries should be directed to Ellen O. Feinberg, (515) 294-3877.

MATERIALS PREPARATION CENTER (continued)

TECHNICAL DATA

MATERIALS

Scandium	Titanium	Magnesium	Thorium
Yttrium	Vanadium	Calcium	Uranium
Lanthanum	Chromium	Strontium	
Cerium	Manganese	Barium	
Praseodymium	Zirconium		
Neodymium	Niobium		
Samarium	Molybdenum		
Europium	Hafnium		
Gadolinium	Tantalum		
Terbium	Tungsten		
Dysprosium	Rhenium		
Holmium			
Erbium			
Thulium			
Ytterbium			
Lutetium			

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt, Director (515) 294-5236
Materials Preparation Center
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

NATIONAL CENTER FOR ELECTRON MICROSCOPY

Lawrence Berkeley Laboratory
University of California
Berkeley, California · 94720

The National Center for Electron Microscopy (NCEM) was formally established in the Fall of 1981 as a component of the Materials and Molecular Research Division, Lawrence Berkeley Laboratory.

The NCEM provides unique facilities and advanced research programs 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 with 1.5 angstrom point-to-point (AMR), a 200-kV high-resolution feeder microscope (JEOL 200 CX), and a 200-kV analytical microscope (JEOL 200 CX) equipped with a thin window and a high-angle X-ray detector, and an energy-loss spectrometer. Facilities for image simulation, analysis and interpretation are also available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. J. J. Hren, Chairman, D. G. Howitt, R. Geiss, D. J. Smith, T. L. Hayes, C. W. Allen, M. M. Treacy, and L. E. Thomas; internal members are G. Thomas, K. M. Krishnan, U. Dahmen, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be of sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer, and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Gretchen Hermes
National Center for Electron Microscopy
Mail Stop: 72-150
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

(510) 486-5006 or
FTS 451-5006

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, cold, straining stages, CBED, video camera.	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. LaB_6 filament. Max. beam current 70 amp/cm^2. 3-mm diameter specimens.
JEOL 1-MeV Atomic Resolution Microscope	Resolution < 1.5 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, ±40° biaxial tilt with height control.	50-80 hrs/week, 400 kV-1 MeV, LaB_6 filament, 3-mm diameter specimens.
Hitachi 650-kV Electron Microscope	General purpose resolution 20 Å environmental cell, straining stage.	Installed in 1969. Max. voltage 650 kV conventional HVEM, 3-mm diameter specimens.
JEOL 200 CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only.	200 kV only, LaB_6 filament, 2.3-mm or 3-mm diameter specimens.
JEOL 200 CX dedicated Analytical Electron Microscope	Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, EELS spectrometer.	100 kV-200 kV LaB_6 filament, state-of-the-art resolution; 3-mm diameter specimens.

DOE CENTER OF EXCELLENCE FOR THE SYNTHESIS AND PROCESSING OF ADVANCED MATERIALS

SANDIA NATIONAL LABORATORIES
ALBUQUERQUE, NEW MEXICO 87185

MEMBER LABORATORIES

Ames Laboratory, Argonne National Laboratory, Brookhaven National Laboratory, University of Illinois Materials Research Laboratory, Lawrence Berkeley Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest Laboratory, Sandia National Laboratories.

OBJECTIVE

The overall objective of this newly-established Center is to enhance synthesis and processing in the DOE with the objective of developing and commercializing new advanced materials.

Synthesis and processing (S&P) are those essential elements of materials science and engineering (MS&E) that deal with the assembly of atoms or molecules to form materials, the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and the development of processes to produce materials for specific applications. Clearly, S&P represent a large area of MS&E that spans the range from fundamental research to applied technology. The goal of basic research in this area ranges from the creation of new materials and the improvement of the properties of known materials, to the understanding of such phenomena as a diffusion, crystal growth, sintering, phase transitions, etc., in relation to S&P. On the applied side, the goal of S&P is to translate scientific results into useful materials by developing processes capable of producing high quality, low-cost products.

APPROACH

The Center's approach is to:

1. Support innovative, fundamental S&P research.
2. Emphasize the concurrent development of S&P including processing equipment and new instruments and techniques for real-time analysis and control.
3. Capitalize on the diverse interdisciplinary science and engineering expertise of the member laboratories.
4. Established partnerships among the Laboratories and Universities to capitalize on those strengths of Universities which complement and reinforce the Center's objectives.
5. Establish partnerships between the DOE labs and industry to demonstrate the ability to shorten the time between the generation and application of MS&E knowledge, to insure the selection of problems of genuine commercial value and to insert the technology into commercial manufacturing concerns.
6. Document the principles learned, the advances made and the remaining barriers.

THE SYNTHESIS AND PROCESSING OF ADVANCED MATERIALS (continued)

In this approach, the emphasis will be on making the processes of basic research, development and applications engineering more concurrent, interactive and overlapping.

FOCUS AREAS

1. Atomically-Structured Materials
2. Complex Polymer Systems
3. Advanced Ceramics and Ceramic Thin Films
4. Nanophase Materials
5. Emerging Materials and Processes

PERSON TO CONTRACT FOR INFORMATION

Geroge A. Samara
Condensed Matter Research Department, 1150
Sandia National Laboratories
Albuquerque, New Mexico 87185

(505) 844-6653
FTS 844-6653

SECTION F

Summary of Funding Levels

SUMMARY OF FUNDING LEVELS

During the fiscal year ending September 30, 1991, the Materials Sciences total support level amounted to about $198.7 million in operating funds (budget outlays) and $17.8 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)	36.2	29.7
(b) South................... (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	10.2	12.5
(c) Midwest................. (IA, IL, IN, MI, MN, MO, OH, WI)	28.8	28.6
(d) West.................... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	24.8	29.2
	100.0	100.0

2. By Discipline:

	Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-)	56.8	26.3
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	32.4	23.9
(c) Materials Chemistry (Budget Activity Numbers 03-)	10.8	9.2
(d) Facility Operations	—	40.6
	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)	29.6
(b) DOE Laboratory Research Programs	28.5
(c) Major Facilities at DOE Laboratories	40.6
(d) Industry and Other	1.3
	100.0

4. By Laboratory and Contract and Grant Research:

	Total Program (%)
Ames Laboratory	5.0
Argonne National Laboratory	19.4
Brookhaven National Laboratory	26.9
Idaho National Engineering Laboratory	0.2
Illinois, University of (Materials Research Laboratory)	3.2
Lawrence Berkeley Laboratory	13.4
Lawrence Livermore National Laboratory	0.9
Los Alamos National Laboratory	6.3
Oak Ridge National Laboratory	17.3
Pacific Northwest Laboratory	1.5
Sandia National Laboratory	4.5
Solar Energy Research Institute	0.2
Stanford Synchrotron Radiation Laboratory	1.2
Contract and Grant Research	
	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 1991 were $228,127,000. The number of projects is 448.

MATERIALS

Actinides-Metals, Alloys and Compounds

6, 15, 32, 34, 35, 52, 128, 134, 147, 152, 163, 219, 231, 281, 325, 362, 386
(1.05, 0.62, 3.79)

Aluminum and Its Alloys

7, 18, 42, 64, 69, 79, 81, 112, 114, 115, 134, 150, 167, 179, 213, 229, 261, 262, 276, 329, 343, 401, 422, 425, 426, 441
(1.65, 0.64, 5.80)

Alkali and Alkaline Earth Metals and Alloys

4, 42, 58, 265, 426
(0.33, 0.19, 1.12)

Amorphous State: Liquids

39, 56, 97, 103, 137, 189, 212, 252, 292, 295, 296, 341, 366, 383, 414
(0.98, 0.52, 3.35)

Amorphous State: Metallic Glasses

19, 24, 29, 53, 67, 69, 91, 112, 119, 142, 149, 163, 167, 172, 179, 202, 212, 242, 288, 334, 397, 441
(1.21, 1.09, 4.91)

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

30, 35, 74, 86, 175, 178, 202, 212, 215, 216, 225, 263, 291, 296, 305, 340, 410
(0.78, 0.79, 3.79)

Amorphous State: Non-Metallic Glasses (Silicates)

16, 35, 84, 147, 195, 200, 212, 216, 230, 283, 291, 296, 305, 334, 376, 394, 410
(1.16, 0.78, 3.79)

Carbides

16, 74, 77, 110, 134, 136, 139, 147, 174, 176, 181, 186, 188, 216, 225, 251, 256, 279, 334, 343, 403, 416, 422, 448
(1.05, 0.80, 5.36)

TECHNIQUES

Electron Spectroscopy for Chemical Analysis (ESCA)

22, 31, 33, 42, 58, 74, 75, 76, 79, 104, 105, 110, 130, 139, 147, 150, 175, 256, 433
(0.67, 0.53, 4.24)

Electron Spin Resonance or Electron Paramagnetic Resonance

40, 85, 116, 119, 158, 176, 205, 207, 260, 273, 311, 317, 361
(0.54, 0.51, 2.90)

Extended X-Ray Absorption Fine Structure (EXAFS and XANES)

22, 33, 34, 48, 49, 60, 74, 84, 126, 147, 163, 212, 219, 256, 262, 285, 340, 344, 410, 411, 413, 428, 429, 430
(1.18, 0.86, 5.36)

Field Emission and Field Ion Microscopy

23, 26, 71, 162, 164, 201, 206, 341
(0.42, 0.35, 1.79)

High Pressure (Technique development of all types)

12, 30, 41, 124, 152, 153, 154, 158, 189, 207, 441
(0.58, 0.41, 2.46)

Ion or Molecular Beams

24, 40, 42, 43, 67, 75, 116, 154, 160, 167, 170, 178, 183, 185, 187, 208, 221, 233, 242, 243, 282
(0.89, 0.96, 4.69)

Ion Channeling, or Ion Scattering (including Rutherford and other ion scattering methods)

24, 27, 29, 42, 67, 70, 79, 81, 116, 145, 167, 170, 175, 176, 183, 184, 187, 202, 218, 233, 234, 314
(1.16, 1.64, 4.91)

Internal Friction (also see Ultrasonic Testing and Wave Propagation)

89, 149, 260, 269, 372
(0.20, 0.04, 1.12)

Infrared Spectroscopy (also see Raman Spectroscopy)

40, 41, 85, 120, 123, 127, 139, 153, 158, 174, 175, 178, 195, 200, 202, 209, 215, 256, 260, 290, 303, 312, 335, 402
(1.16, 0.72, 5.36)

Laser Spectroscopy (scattering and diagnostics)

42, 43, 122, 123, 124, 129, 138, 144, 153, 160, 178, 189, 193, 197, 203, 204, 208, 209, 211, 252, 263, 277, 283, 291, 332, 336, 339, 366, 369, 383, 398, 407, 412, 418, 435
(2.10, 0.89, 7.81)

Magnetic Susceptibility

6, 12, 13, 25, 31, 32, 38, 51, 119, 140, 145, 152, 154, 155, 177, 185, 205, 207, 231, 253, 281, 286, 311, 317, 361, 382, 409
(1.83, 1.27, 6.03)

Theory: Defects and Radiation Effects

27, 36, 50, 64, 65, 67, 141, 145, 147, 156, 158, 167, 180, 196, 219, 225, 235, 243, 260, 272, 287, 314, 332, 340, 353
(1.54, 3.29, 5.58)

Theory: Electronic and Magnetic Structure

6, 19, 22, 25, 33, 35, 36, 40, 41, 47, 57, 94, 109, 125, 127, 134, 143, 152, 156, 158, 161, 166, 180, 204, 205, 210, 216, 220, 237, 254, 273, 280, 281, 283, 287, 289, 303, 325, 330, 331, 334, 362, 364, 365, 381, 386, 419, 421, 424, 431
(2.95, 1.58, 11.16)

Theory: Non-Destructive Evaluation

7, 223, 359
(0.22, 0.09, 0.67)

Theory: Surface

36, 42, 47, 57, 65, 71, 87, 94, 117, 125, 126, 139, 156, 160, 161, 166, 180, 195, 201, 210, 228, 235, 239, 248, 288, 289, 310, 324, 346, 347, 355, 357, 379, 381, 384, 419, 421, 436
(2.30, 1.12, 8.48)

Theory: Structural Behavior

4, 6, 18, 97, 109, 110, 114, 125, 156, 157, 160, 161, 168, 171, 200, 222, 245, 249, 259, 261, 265, 267, 269, 279, 287, 289, 303, 315, 319, 321, 322, 324, 325, 327, 329, 336, 342, 343, 345, 350, 355, 357, 372, 378, 380, 387, 397, 399, 400, 403, 407, 419, 425, 427, 435
(4.35, 1.57, 12.28)

Theory: Superconductivity

17, 28, 32, 35, 50, 57, 94, 118, 119, 125, 127, 152, 154, 156, 166, 180, 185, 205, 220, 281, 319, 334, 345, 362, 409, 420, 424, 431
(1.85, 1.25, 6.25)

Theory: Thermodynamics, Statistical Mechanics, and Critical Phenomena

39, 47, 57, 94, 97, 109, 114, 119, 127, 129, 134, 142, 149, 155, 156, 157, 160, 161, 168, 178, 180, 189, 190, 191, 210, 230, 236, 237, 248, 259, 261, 265, 273, 280, 287, 288, 307, 319, 324, 347, 372, 390, 415, 430
(2.19, 1.40, 9.82)

Theory: Transport, Kinetics, Diffusion

2, 3, 25, 40, 50, 66, 67, 71, 114, 131, 133, 136, 166, 167, 178, 180, 189, 192, 204, 210, 224, 225, 230, 236, 237, 241, 245, 254, 260, 269, 272, 287, 288, 312, 319, 326, 328, 334, 347, 348, 356, 365, 373, 374, 375, 381, 383, 386, 390, 400, 404
(2.92, 1.45, 11.38)

Thermal Conductivity

91, 155, 192, 408
(0.45, 0.16, 0.89)

Ultrasonic Testing and Wave Propagation

7, 66, 149, 303, 359, 372, 407
(0.33, 0.11, 1.56)

PHENOMENA

Diffusion: Surface

1, 42, 43, 71, 104, 106, 112, 116, 117, 137, 139, 206, 288, 298
(0.67, 0.42, 3.13)

Dislocations

5, 26, 65, 73, 78, 79, 81, 91, 112, 114, 115, 116, 148, 150, 162, 164, 167, 204, 210, 224, 247, 269, 270, 275, 349, 397, 405, 417
(1.14, 0.61, 6.25)

Dynamic Phenomena

35, 36, 52, 119, 122, 124, 137, 155, 172, 173, 180, 191, 199, 211, 213, 228, 238, 263, 277, 282, 288, 291, 303, 326, 333, 372, 383, 389, 392, 398, 412, 418, 436
(1.96, 1.41, 7.37)

Electronic Structure - Metals including amorphous forms

1, 15, 19, 20, 22, 32, 34, 35, 56, 58, 93, 98, 112, 125, 127, 134, 137, 143, 152, 154, 156, 161, 166, 180, 210, 212, 241, 242, 258, 278, 280, 283, 287, 325, 334, 338, 344, 358, 362, 368, 381, 386, 413, 424, 434
(2.30, 1.78, 10.04)

Electronic Structure - Non-metals including amorphous forms

19, 25, 33, 56, 74, 75, 93, 103, 122, 125, 137, 154, 156, 158, 160, 161, 195, 209, 220, 237, 253, 254, 259, 262, 263, 286, 291, 331, 332, 334, 342, 347, 353, 365, 368, 409, 418, 427
(2.19, 0.76, 8.48)

Erosion

343
(0.00, 0.00, 0.22)

Grain Boundaries

2, 5, 8, 26, 37, 48, 49, 51, 64, 65, 73, 79, 81, 86, 110, 112, 116, 143, 148, 150, 156, 162, 164, 166, 167, 171, 181, 182, 194, 196, 210, 213, 216, 226, 234, 243, 264, 267, 269, 270, 275, 276, 278, 302, 307, 309, 310, 320, 322, 324, 338, 342, 351, 355, 359, 360, 374, 380, 389, 403, 405, 416, 433
(2.88, 1.83, 14.06)

Hydrogen Attack

77, 78, 79, 81, 153, 202, 221, 322, 360
(0.49, 0.22, 2.01)

Ion Beam Mixing

24, 27, 29, 42, 67, 116, 167, 170, 183, 184, 188, 225, 242, 243
(0.78, 1.50, 3.13)

Laser Radiation Heating (annealing, solidification, surface treatment)

42, 66, 75, 144, 146, 153, 178, 181, 183, 184, 202, 288, 292, 398
(0.80, 1.01, 3.13)

Radiation Effects (use specific effects, e.g., Point Defects and Environment Index)

5, 27, 29, 37, 42, 67, 90, 118, 145, 147, 162, 164, 167, 180, 181, 182, 197, 217, 229, 242, 243, 314, 332, 340
(1.34, 0.96, 5.36)

Recrystallization and Recovery

84, 97, 114, 184, 197, 340, 380
(0.54, 0.19, 1.56)

Residual Stress

7, 63, 150, 279, 318, 371, 407
(0.56, 0.19, 1.56)

Rheology

88, 129, 200, 366, 387, 402
(0.56, 0.31, 1.34)

Stress-Corrosion

41, 49, 66, 68, 78, 146, 194, 196, 201, 300, 322, 328, 330, 360, 394
(0.94, 0.55, 3.35)

Solidification (conventional)

2, 9, 169, 236, 244, 252, 257, 375
(0.31, 0.17, 1.79)

SOL-GEL Systems

85, 147, 168, 179, 185, 200, 366, 376
(0.54, 0.45, 1.79)

Solidification (rapid)

2, 30, 64, 69, 180, 184, 213, 236, 292, 313, 382, 430
(0.69, 0.46, 2.68)

Surface Phenomena: Chemisorption (binding energy greater than 1eV)

1, 15, 43, 58, 68, 76, 93, 98, 104, 105, 106, 117, 125, 131, 133, 135, 136, 137, 138, 139, 166, 186, 201, 217, 221, 227, 228, 239, 288, 294, 301, 341, 346, 357, 368, 369, 396, 410, 413, 423, 430, 436
(2.39, 1.12, 9.38)

Surface Phenomena: Physiosorption (binding energy less than 1eV)

18, 31, 42, 55, 58, 59, 68, 104, 105, 120, 137, 139, 186, 201, 206, 227, 244, 357, 369, 393
(1.23, 0.93, 4.46)

Surface Phenomena: Structure

13, 18, 34, 36, 40, 49, 55, 71, 73, 76, 87, 95, 98, 105, 106, 121, 125, 130, 131, 137, 138, 139, 161, 165, 180, 186, 194, 210, 217, 228, 234, 248, 268, 271, 282, 285, 295, 324, 341, 355, 357, 371, 381, 389, 410, 411, 413, 423, 427, 436, 438
(2.70, 1.29, 11.38)

Gas: Oxidizing

26, 81, 110, 148, 153, 154, 171, 194, 201, 210, 217, 227, 298, 299, 313, 329, 388
(1.76, 1.52, 3.79)

Gas: Sulphur-Containing

301, 329
(0.22, 0.06, 0.45)

High Pressure

12, 14, 19, 41, 52, 53, 54, 103, 124, 128, 139, 153, 154, 192, 204, 224, 231, 259, 266, 367, 378, 388, 428
(2.32, 1.72, 5.13)

Magnetic Fields

6, 12, 17, 25, 28, 32, 45, 50, 52, 53, 59, 114, 119, 128, 141, 154, 177, 231, 240, 253, 255, 424
(2.32, 4.74, 4.91)

Radiation: Electrons

90, 107, 108, 113, 118, 141, 145, 147, 197, 217, 225, 301, 314, 353, 393, 444
(2.05, 2.45, 3.57)

Radiation: Gamma Ray and Photons

14, 34, 38, 42, 45, 46, 141, 144, 145, 147, 165, 192, 196, 225, 291, 332, 410, 442, 443, 444, 447
(2.48, 5.24, 4.69)

Radiation: Ions

42, 43, 67, 145, 147, 154, 167, 170, 177, 183, 184, 196, 197, 202, 219, 233, 242, 243, 286, 314, 318, 340
(3.10, 2.56, 4.91)

Radiation: Neutrons

5, 37, 38, 67, 97, 145, 147, 165, 167, 185, 192, 196, 197, 403
(1.27, 1.32, 3.13)

Radiation: Theory (use Theory: Defects and Radiation Effects in the Techniques Index)

27, 67, 167, 197, 314
(0.49, 0.93, 1.12)

Temperatures: Extremely High (above 1200degK)

3, 5, 9, 11, 12, 21, 25, 26, 30, 54, 55, 82, 110, 123, 134, 148, 153, 154, 162, 171, 188, 209, 211, 222, 224, 226, 259, 272, 292, 310, 348, 367, 403, 410, 416, 417, 446
(5.33, 3.49, 8.26)

Temperatures: Cryogenic (below 77degK)

6, 11, 12, 17, 25, 30, 31, 32, 37, 38, 40, 50, 51, 52, 53, 54, 55, 58, 90, 91, 97, 98, 102, 114, 118, 119, 124, 127, 128, 139, 153, 154, 155, 160, 177, 192, 204, 218, 231, 240, 244, 253, 294, 310, 348, 385, 410
(5.78, 5.28, 10.49)

Vacuum: High (better than 10**9 Torr)

9, 15, 25, 31, 34, 42, 43, 45, 46, 55, 56, 71, 73, 87, 93, 95, 105, 138, 139, 141, 143, 144, 149, 183, 186, 201, 206, 268, 282, 298, 398, 423
(4.29, 7.62, 7.14)

MAJOR FACILITIES: OPERATIONS

Pulsed Neutron Sources (Operations)

44, 151, 159
(0.67, 6.03, 0.67)

Steady State Neutron Sources (Operations)

61, 192, 395
(0.67, 11.17, 0.67)

Synchrotron Radiation Sources (Operations)

34, 62, 121, 201, 262, 325, 429
(1.56, 7.59, 1.56)